ENGINEERING CHANGE NOTICE

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Page 1 of 5

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13a. Description of Change Changes to text noted with margin bars. Details of code changes noted below. <u>Major Code Changes</u> 1. Allow axial nodalization of fuel elements and consider conduction along the fuel elements to track axial temperature profile. Allow non-uniform distribution of the oxidation area, surface water mass, wetted fraction of the surface and sludge mass along the fuel elements. Radiation and micro-convection with adjacent fuel elements should be done on an axial node basis. Corrosion and evaporation/condensation should be determined for each individual axial node. (See continuation pages)							
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14b. Justification Details Code changes required for more accurate physical modeling and efficiency							
15. Distribution (include name, MSIN, and no. of copies) See Distribution Sheet							

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ENGINEERING CHANGE NOTICE CONTINUATION SHEET

Page 3 of 5

ECN 652260

Date 03/10/99

2. Allow axial nodalization of scrap basket and consider conduction along the vertical axis. Allow non-uniform distribution of the porosity, oxidation area, and water content.

Errors Corrected

3. The code dies when initial region gas temperature of 25 C is specified.
4. The code dies when a region is filled with 100% steam.
5. The steam does not condense on the inner surface of the MCO wall adjacent to the scrap basket.
6. The molecular weight ratio of the hydride to the uranium oxide should be 241/270, not 241/238.
7. The coefficients of discretized equations for cylindrical heat sinks are incorrect.
8. Incorrect hydrogen generation rate when liquid water reacts with fuel.
9. Minor error in determining the average heat sink temperature.
10. Limitation of the heat diversion model.
11. Fuel temperature printout ceiling of 999.9°C
12. Truncated input file name.
13. Error in the scrap radiation model.
14. Error in the temperature dependent emissivity feature.
15. Lower peak scrap temperature.
16. Leaking check valve.
17. Non-zero hydride oxidation area after hydride depletion.
18. Hydrogen accumulation without time step initialization.
19. Scrap basket water axial fraction error.
20. MCO wall axial conduction distance incorrectly divided.

Input/Output Changes

21. Allow the restart file name to be specified in the input deck.
22. Make I/O routines generic so that the code can be compiled with non-Lahey FORTRAN compilers.
23. Introduce control flags so that only desired set of heat sink temperatures are printed out in the output and in the log files.

ENGINEERING CHANGE NOTICE CONTINUATION SHEET

Page 4 of 5

ECN 652260

Date 03/10/99

24. Include the axial temperature profile of fuel elements in the MCO specific output.
25. Previously, much of the same information had to be repeated for each fuel basket input section, such as the view factor and the conduction distance matrices. Introduce a way to circumvent repeating the same information in the input deck.
26. Detect unrecognizable key words in the input deck and print out informative message to the log file before terminating the program.
27. In the MCO specific summary output, right after the uranium mass, print out the total heat capacity of fuel and structure material in MCO, with and without the cask, including the liquid water on the surface. The heat capacities of the MCO wall, shield plug, and the cask are printed only once at the beginning of the run. Also, add a column in the MCO specific summary output for the total over all baskets for uranium mass, water mass, reaction area, etc.
28. Print out the hydride oxidation area.
29. Labels for heat sink temperature plot variables will be able to accommodate three-digit heat sink number: for example, THSA101.
30. Do not double count duplicate plot variables. It affects the total number of plot variables that gets printed at the top of the *.PLT file.

Enhancement of Current Features

31. Allow heat sinks to have single internal node, i.e. lumped heat sink.
32. Track water on the insert of scrap and fuel baskets.
33. The corrosion rate of water covered portion of the fuel surface will be based on the saturation pressure at the fuel temperature, not on the partial pressure of steam in the free steam. Such reaction should consume water on the fuel surface not the steam in the free stream.
34. Add third option to flag IHYDKP (a control flag to suppress depletion of hydride as it oxidizes) to keep the rate multiplier the same, but deplete hydride mass as it reacts and stop reaction when the mass is zero. Also, for IHYDK = 1 option, perform a phantom calculation of hydride mass depletion, but continue to the constant rate multiplier even when the mass gets to zero. The last option will be used by the analyst to determine how long it takes to consume all hydrides.
35. Increase the number of regions that can be modeled from 7 to 10.
36. For the alternative rate law option (i.e. ILAW=1), Trimble's correlation will be used for the dry air temperature less than 300 C. That is,
- $$10^{(7.19-3732/T)} \text{ mg-O}_2/\text{cm}^2/\text{hr}$$
37. Provide a smooth transition between the mass diffusion controlled evaporation/condensation rate to the boiling controlled rate when the fuel temperature increased.

New Features

38. Add fan junctions (provide an option to model either a constant P fan or a constant volumetric displacement pump).
39. Add a capability to model check valves, with dead-bands, and failure junctions. Also, keep track of the time each check valve junction remained open and print it out to the summary of the output file.
40. Consider conduction heat transfer along the contiguous insert and to the shield plug.
41. Allow a group of heat sinks to exchange radiation heat based on the user specified view factor matrix.
42. Allow sandwiched heat sinks.
43. Introduce material library for the heat sink.
44. Introduce a multiplier for thermal conductivity of the region gas.

Mass/Energy Balance Feature

45. Print out and plot energy balance in MCO

Code Architecture

46. Move determination of the surface areas and volumes of heat sinks from subroutine MCO to subroutine HSINI.
47. Introduce temperature dependent emissivity of heat sink surfaces.
48. Entrainment of fluffy freshly oxidized UO_2 , instead of the sludge particles, which is believed to be strongly adhered to the surface after washing, should be considered.
49. Make the gas conductivity multiplier region specific.
50. Introduce multipliers for the effective thermal conductivity of the scrap basket, excluding the radiation component.

DISTRIBUTION SHEET

To	From	Page 1 of 1
SNF 3650, Rev. 1 Distribution	Process Engineering	Date 02/26/99
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HANSF 1.3 USER'S MANUAL

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Abstract: The HANSF analysis tool is an integrated model considering phenomena inside a multi-canister overpack (MCO) spent nuclear fuel container such as fuel oxidation, convective and radiative heat transfer, and the potential for fission product release. It may be used for all phases of spent fuel disposition including cold vacuum drying, transportation, and storage. This manual reflects HANSF version 1.3, a revised version of version 1.2a. HANSF 1.3 was written to add new models for axial nodalization, add new features for ease of usage, and correct errors. HANSF 1.3 is intended for use on personal computers such as IBM-compatible machines with Intel processors running under a DOS-type operating system. HANSF 1.3 is known to compile under Lahey TI and Digital Visual FORTRAN, Version 6.0, but this does not preclude operation in other environments.

This manual also incorporates minor errors (8-20 on page 3 of ECN Continuation Sheet) for the minor code revision HANSF 1.3.1.

*Fauske and Associates, Inc., Burr Ridge, Illinois

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TABLE OF CONTENTS

	<u>Page</u>
LIST OF FIGURES	vi
LIST OF TABLES	ix
LIST OF REVISION 2 CHANGE PAGES	x
 1.0 PURPOSE AND BACKGROUND	 1-1 of 49
1.1 Scope	1-1
1.2 Uranium Oxidation and Pyrophoricity	1-2
1.2.1 Oxidation Rate Data	1-2
1.2.2 Air Oxidation of N-Reactor Fuel	1-5
1.2.3 Ignition Theory	1-11
1.2.4 Experimental Basis	1-12
1.2.5 Application to MCO Analysis	1-16
1.3 Fission Product Release	1-16
1.3.1 Experimental Basis	1-16
1.3.2 Application to MCO Analysis	1-20
1.4 Uranium Oxide Hydrate Decomposition	1-20
1.4.1 Unirradiated Material Data	1-20
1.4.2 K-Basins Sludge Water Content and Dehydration Characterization Data	 1-21
1.4.3 Application to MCO Analysis	1-25
1.5 Aerosol Transport and Deposition	1-25
1.5.1 Experimental Basis	1-25
1.5.2 Application to MCO Analyses	1-26
1.6 Counter-Current Flow	1-26
1.6.1 Experimental Basis	1-26
1.6.2 Application to MCO Analysis	1-28
1.7 Nitriding	1-30
1.7.1 Experimental Basis	1-30
1.7.2 Application to MCO Analysis	1-31
1.8 Copper Corrosion	1-32
1.8.1 Experimental Basis	1-32
1.8.2 MCO Application	1-33

TABLE OF CONTENTS (continued)

	<u>Page</u>
1.9 Uranium Hydrides	1-33
1.9.1 MCO Application	1-37
1.10 Natural Circulation Inside the MCO	1-37
1.10.1 Experimental Basis	1-37
1.10.2 Application to MCO Analysis	1-40
1.11 Reactive Area Distribution	1-40
1.11.1 Fuel Element Axial Temperature Profile	1-40
1.11.2 Application to MCO Analysis	1-47
2.0 REGION AND TRANSPORT MODELS	2-1 of 25
2.1 Model Structure	2-1
2.2 Region Thermodynamics	2-2
2.3 Heat Transfer	2-4
2.3.1 Finite Difference Solution for Heat Sink Temperature	2-4
2.3.1.1 Discretization For Interior Nodes	2-5
2.3.1.2 Discretization For Boundary Nodes	2-8
2.3.1.3 Discretization For Composite Heat Sinks	2-10
2.3.2 Heat Transfer to Heat Sink Surfaces	2-11
2.4 Aerosol Model	2-14
2.5 Gas Flow Model	2-16
2.6 Counter-Current Flow	2-17
2.6.1 Horizontal Walls	2-18
2.6.2 Vertical Walls	2-19
2.6.3 Combined Forced and Natural Convection Flow in Horizontal Walls	2-20
2.6.4 Combined Forced and Natural Convection Flow in Vertical Walls	2-20
2.7 Entrainment	2-20
2.8 De-Entrainment	2-22
2.9 Properties	2-23
3.0 MCO MODELS	3-1 of 53
3.1 MCO Description	3-1

TABLE OF CONTENTS

(continued)

	<u>Page</u>
3.2 Nodalization and Assumptions	3-10
3.3 Oxidation of Fuel	3-14
3.4 Hydriding / Dehydriding	3-24
3.5 Uranium Oxide Hydrate Decomposition	3-25
3.5.1 Assumptions	3-25
3.5.2 Equilibrium and Decomposition Laws	3-26
3.5.3 Decomposition Limitations	3-28
3.6 Heat Transfer in the Fuel Basket	3-29
3.6.1 Radiation Heat Transfer	3-29
3.6.2 Micro-Convection Heat Transfer	3-31
3.6.3 Diversion Heat Transfer to Gas	3-35
3.7 Heat Transfer in the Scrap Basket	3-37
3.7.1 Effective Thermal Conductivity in a Rubble Bed	3-37
3.7.2 Nodalization of Scrap Basket and Treatment of "Fin"	3-37
3.7.3 Diversion Heat Transfer to Gas in Scrap Basket	3-40
3.8 Evaporation and Condensation	3-42
3.8.1 Implicit Method for Steam Partial Pressure	3-47
3.8.2 Implementation in the Code	3-48
3.9 Radiolysis	3-48
3.10 Nitriding	3-52
4.0 CODE ARCHITECTURE	4-1 of 18
4.1 Main Program Organization	4-1
4.2 Subroutine and Function Descriptions	4-4
4.3 Subroutine and Function Calls	4-9
5.0 INPUT DESCRIPTION	5-1 of 46
5.1 Species Properties	5-1
5.2 Input File	5-4
5.2.1 CONTROL Section	5-5
5.2.1.1 TITLE Sub-Section	5-6

TABLE OF CONTENTS

(continued)

	<u>Page</u>
5.2.1.2 TIMING Sub-Section	5-6
5.2.1.3 ACTIVE Sub-Section	5-9
5.2.1.4 SOURCES Sub-Section	5-10
5.2.1.5 PLOTTING Sub-Section	5-12
5.2.1.6 PRINT Sub-Section	5-14
5.2.2 VOLUMES Section	5-15
5.2.3 HEAT_SINKS Section	5-17
5.2.3.1 Basic Inputs	5-18
5.2.3.2 Time-Dependent Boundary Conditions	5-19
5.2.3.3 Material Library	5-20
5.2.3.4 Composite Heat Sinks	5-21
5.2.3.5 Conduction Networks	5-21
5.2.3.6 Radiation Networks	5-22
5.2.3.7 Temperature-Dependent Emissivity	5-23
5.2.4 JUNCTIONS Section	5-23
5.2.5 MCO Section	5-27
5.2.5.1 GENERAL Sub-Section	5-28
5.2.5.2 SOLAR RADIATION Sub-Section	5-32
5.2.5.3 FUEL_BSKT Sub-Section	5-33
5.2.5.4 SCRAP_BSKT Sub-Section	5-39
5.2.5.5 MCO Plotting Sub-Section	5-42
6.0 OUTPUT DESCRIPTION	6-1 of 12
6.1 Log File	6-1
6.2 Plot File	6-2
6.3 Tabular Output File	6-5
6.4 Restart File	6-11
6.5 MCO-Specific Plot File	6-11
7.0 SEPARATE EFFECTS TESTING	7-1 of 45
7.1 Region Thermodynamics	7-1
7.2 Fog Formation	7-2

TABLE OF CONTENTS
(concluded)

	<u>Page</u>
7.3 Inter-Compartmental Flow	7-3
7.4 Heat Sink Modeling	7-6
7.5 Aerosol Transport and Deposition	7-9
7.5.1 Sedimentation	7-9
7.5.2 Leakage	7-11
7.6 Counter-Current Flow	7-12
7.7 De-Entrainment	7-17
7.8 Evaporation/Condensation Validation	7-18
7.9 Hydriding/Dehydriding Validation	7-24
7.10 Uranium Oxidation Validation	7-25
7.11 Entrainment Validation	7-27
7.12 Hydrate Decomposition Validation	7-28
7.13 Heat Transfer Validation	7-31
7.13.1 Fuel to Gas Heat Transfer	7-31
7.13.2 Scrap Basket Heat Transfer	7-32
7.14 Nitriding Validation	7-35
7.15 Pump Model	7-36
7.16 Radiation Network Validation	7-39
7.17 Energy Balance Validation	7-41
8.0 INTEGRAL TESTING	8-1 of 7
8.1 Cold Vacuum Drying	8-1
8.2 Shipping Calculation	8-3
8.3 Interim Storage	8-5
8.4 Cold Vacuum Drying With Axial Variation in Fuel Damage	8-6
9.0 REFERENCES	9-1 of 4
APPENDIX A Input Decks for Separate Effects	A-1 of 113
APPENDIX B Sample Problem Input	B-1 of 37
APPENDIX C Sample Problem Output	C-1 of 14
APPENDIX D Quality Assurance Documents	D-1 of 4

LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
1-1	Rates of Reaction (rate of weight gain of O_2) at 100% RH in the $U-H_2O$ and $U-O_2-H_2O$ Systems	1-3
1-2	Effect of Oxygen Concentration on the Reaction Rate of Uranium at 100°C in the $U-O_2-H_2O$ System, Total Pressure 10 kPa	1-4
1-3	Variation of Gas Composition With Time in $U-O_2-H_2O$ Experiments	1-6
1-4	Uranium Oxidation Rate Law Comparison	1-7
1-5	PNNL Uranium-Air TGA Detail	1-8
1-6	PNNL Uranium-Air TGA Run 18 and 49b Slopes	1-9
1-7	Comparison of SNF Oxidation Rate in Dry Air to Literature Data	1-10
1-8	Tetenbaum's Experimental Apparatus	1-13
1-9	Crucible Wall Ignition Temperature Versus Uranium Powder Height in Different Diameter Crucibles - Ignition Theory Compared With Experimental Data of Tetenbaum, et al., [1962]	1-14
1-10	Crucible Wall Ignition Temperature Versus Uranium Powder Height in Different Diameter Crucibles - Ignition Theory Compared With Experimental Data of Tetenbaum, et al., [1962]	1-15
1-11	Effect of Temperature on Release of Iodine, Tellurium, and Xenon	1-18
1-12	UO_3-H_2O Drying Curve	1-22
1-13	Containment Systems Test Facility for Test AB-5 and Test Results for Suspended Mass	1-27
1-14	Pure Counter-Current Flow Through a Rectangular Flowpath in a Horizontal Wall, i.e., Vertical Flow	1-29
1-15	Decomposition Pressure vs. Temperature for UH_3	1-35
1-16	The Temperature Dependence of the Reaction Front Velocity U for Two Working Pressures	1-36

LIST OF FIGURES

(continued)

<u>Figure</u>	<u>Page</u>
1-17	Nusselt Number for Natural Circulation in an Annular Porous Layer 1-39
1-18	Axial Temperature Difference as a Function of Ambient Temperature for Heat Rejection, for Various Rate Enhancement Factors vs. Literature Data to Represent Surface Area Increases Due to Roughness, Cracking, or Hydrides, and for Various Steam Partial Pressures 1-46
1-19	Marginal Rate Law Enhancement Factor as Function of Ambient Temperature for Heat Rejection, for Various Steam Partial Pressures in kPa 1-48
2-1	Interior Heat Sink Node Discretization 2-6
2-2	Boundary Half-Nodes 2-9
2-3	Composite Heat Sink 2-12
3-1A	MCO Top Portion With Shield Plug and Cover 3-2
3-1B	MCO Bottom Portion 3-3
3-2	MCO Shield Plug 3-4
3-3	Mark IV Fuel Basket 3-5
3-4	Base Plate Assembly and Dimensions 3-6
3-5A	Scrap Basket Configuration 3-7
3-5B	Scrap Basket Configuration 3-8
3-6	MCO Control Volumes and Flowpaths 3-11
3-7	Pin-by-Pin Nodalization Scheme 3-12
3-8	Sample Scrap Basket Nodalization 3-13
3-9	Oxidation Rate Law Logic 3-19

LIST OF FIGURES

(concluded)

<u>Figure</u>		<u>Page</u>
3-10	Flowchart for Radiation Heat Transfer Calculation Between Fuel Elements, the MCO Wall, and the Insert	3-33
3-11	Flowchart for Heat Transfer Calculation in the Scrap Basket	3-41
3-12	Flowchart for Evaporation/Condensation Rate Calculation	3-49
3-13	Flowchart for Subroutine EVPCND (IMODE = 0)	3-50
3-14	Flowchart for Subroutine EVPCND (IMODE = 1)	3-51
4-1	HANSF Main Program Flowchart	4-2
5-1	Gas Properties Set for Nitrogen	5-2
7-1	Pressure History for Ideal Gas Source and Outflow Test Case	7-5
7-2	Suspended Mass History for AB-5 Data and Prediction	7-10
7-3	Output for Aerosol Leakage Validation	7-13
7-4	Counter-Current Flow Rate Through Junction	7-14
7-5	Compartment Temperatures for Counter-Current Flow Validation	7-15
7-6	Aerosol De-Entrainment Model Validation Test (With 90° Bend)	7-19
7-7	Aerosol De-Entrainment Model Validation Test (Without Bend)	7-20
7-8	Gas Temperature for Heat Transfer Validation	7-33

LIST OF TABLES

<u>Table</u>	<u>Page</u>
1-1 Summary of Hilliard's Experimental Conditions	1-19
1-2 Drying Results of the Last Seven KE Canister Sludge Samples	1-24
1-3 Interpreted Canister Sludge Dryout Results	1-24
1-4 Calculation of Axial Temperature Difference	1-45
3-1 Key Fuel and MCO/Cask Dimensions	3-9
3-2 Oxidation Rate Law Summary	3-18
3-3 View Factors For Pin-By-Pin Model	3-32
3-4 Conduction Distance - Pin-by-Pin Model	3-34
3-5 Radiolytic Gas Generation in a Drained/Dried Multi-Canister Overpack	3-52
7-1 Constitutive Relation Validation	7-2
7-2 Fog Formation Sample Problem	7-4
7-3 Test Case Values	7-6
7-4 Comparison of the Semi-Infinite Slab Solution for Surface Temperature with Model Results	7-8
7-5 Comparison of Model Results With Analytical Results Obtained from Heisler Charts	7-9
7-6 Uranium Oxidation Validation	7-26
7-7 Nitriding Validation	7-36
7-8 Mass of Fuel in One Fuel Basket	7-43
8-1 Simulation Input Values for Integral Test Case 1	8-2
8-2 Simulation Input Values for Integral Test Case 4	8-7

LIST OF REVISION 2 CHANGE PAGES

Title Page

Table of Contents (pp. i through v and vii through ix)

Addition of List of Revision 2 Change Pages (this page, x)

Section 2.3.1.1 (pp. 2-5 and 2-7)

Section 2.3.1.2 (pg. 2-10)

Section 2.3.1.3 (pp. 2-11 through 2-13 are affected by repagination)

Section 2.3.2 (pp. 2-14 and 2-15 are affected by repagination)

Figures 3-7 and 3-8 (pp. 3-12 and 3-13)

Section 3.3 (pp. 3-17 through 3-31 are affected by repagination)

Section 3.6.2 (pp. 3-32 through 3-35 are affected by repagination)

Section 3.6.3 (pg. 3-36)

Section 3.7.1 (pp. 3-37 through 3-41 are affected by repagination)

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Section 3.8.1 (pg. 3-47)

Section 3.8.2 (original Section deleted - replaced and renumbered by original Section 3.8.3
pp. 3-48 through 3-53 are affected by repagination)

Section 5.2.1.3 (pp. 5-9 through 5-19 are affected by repagination)

Section 5.2.3.4 (pg. 5-21)

Section 5.2.3.5 (pp. 5-22 through 5-28 are affected by repagination)

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Section 5.2.5.3 (pp. 5-33 through 5-38 are affected by repagination)

LIST OF REVISION 2 CHANGE PAGES
(concluded)

Section 5.2.5.4 (pp. 5-39 through 5-43 are affected by repagination)

Section 5.2.5.5 (pp. 5-44 through 5-46)

Appendix B - Section B.4 (pp. B-24 through B-35)

Appendix B - Section B.5 (pp. B-36 and B-37)

Appendix C - Section C.4 (pp. C-12 through C-14)

Appendix D (pp. D-1 through D-4)

1.0 PURPOSE AND BACKGROUND

1.1 Scope

The HANSF analysis tool is an integrated model considering phenomena inside a multi-canister overpack (MCO) container such as fuel oxidation, convective and radiative heat transfer, and the potential for fission product release. The model accounts generically for such phenomena as gas and aerosol flows between regions (such as between the MCO and an operating area), aerosol agglomeration and deposition, and heat transfer to structures, including condensation. It may be used for all phases of spent fuel disposition including cold vacuum drying, transportation, staging, hot vacuum conditioning, and storage.

The bottom-line goal of the HANSF tool described here is to predict whether or not postulated accident situations could lead to the release of fission products from spent fuel, in particular from a multi-canister overpack (MCO) container holding fuel elements, and to quantify releases of radionuclides from facilities to the site. The analysis tool is "integrated" to incorporate models for a wide variety of phenomena.

The analysis tool described here is useful and practical because it is a small computer program that runs very quickly on a personal computer, and facilitates many simulations in a matter of days. A similar model was successfully used for consequences of accidents at Hanford tank farms [Plys, et al, 1996]; many cases were simulated in a few days on personal computer to investigate sensitivity to input parameters.

Phenomenological capabilities include:

- Multiple-compartment representation (MCO plus all downstream rooms),
- Pressure-driven and counter-current gas flows,
- Transport of gases and aerosols between compartments,

- Vapor-aerosol equilibrium,
- Deposition of aerosols via gravitational sedimentation, impaction, etc.,
- Entrainment of aerosol from deposited particulate,
- Heat transfer and condensation on structures (including fuel), and
- Chemical reactions of fuel including oxidation, hydriding, dehydration, and nitriding.

Integral accident assessment combines models for reaction kinetics (uranium oxidation) with models for temperature distributions in the fuel and other solids, fission product releases, and aerosol and vapor transport and deposition. Each of these considerations is discussed below briefly.

1.2 Uranium Oxidation and Pyrophoricity

1.2.1 Oxidation Rate Data

In the handling and storage of uranium fuels, uranium corrosion is a concern because uranium hydride, which is potentially pyrophoric, and hydrogen may be produced. Uranium oxidation also acts as a chemical heat generation source. The reaction of uranium in oxidizing atmospheres has been investigated extensively. Pearce [Pearce, 1989] compiled the available reaction rate data for unirradiated uranium in atmospheres of dry and moist air, steam, and carbon dioxide; these data span the range between room temperature and the melting point of uranium. Reaction rate data for nitrogen and carbon monoxide are also available, and the enhancing effect of irradiation has been investigated as well.

Rate law equations will be described in the MCO model description. Available data show that the uranium oxidation rate increases greatly with added moisture, and that pure water corrosion exceeds any in which air is present. Figures 1-1 and 1-2 illustrate the influences of temperature and gas composition on oxidation. It is notable that when both oxygen and water

Figure 1-1:
Rates of Reaction (rate of weight gain of O_2) at 100% RH
in the $U-H_2O$ and $U-O_2-H_2O$ Systems [Pearce, 1989].

Figure 1-2: Effect of Oxygen Concentration on the Reaction Rate of Uranium at 100°C in the U-O₂-H₂O System, Total Pressure 10 kPa, from [Pearce, 1989].

vapor are present, net oxygen depletion occurs before net water vapor reactions, as seen in Figure 1-3. For reference, a number of literature correlations are summarized in Figure 1-4.

1.2.2 Air Oxidation of N-Reactor Fuel

Experiments for air oxidation rates of N-reactor fuel were conducted by PNNL [Abrefah, et al., 1998] and have recently been analyzed in detail [Trimble and Welsh, 1998; and Cramer and Abrefah, 1997]. Results are summarized here.

Figure 1-5 contains an illustration of the portion of the thermogravimetric analysis apparatus used by PNNL for its isothermal N-reactor fuel-air oxidation experiments. Experiments were conducted at nominal furnace temperatures between 69°C and 400°C. Results of a typical experiment, here at 150°C, are shown in Figure 1-6 as analyzed by [Trimble and Welsh, 1998]. Four periods of distinct positive weight gain slopes are evident, as are several periods with negative slopes (weight loss). The steepest slope corresponds to a rapid oxidation event. Note that typical sample weights are about 6 grams, typical total weight gains (which depend greatly on temperature) are on the order of tens of milligrams, i.e., on the order of 1% or less, and typical reaction areas are about 2.5 cm².

Figure 1-7 contains a plot of reaction rates for seven experiments selected by [Abrefah, et al., 1998] compared to literature data and correlations. It is evident that these N reactor fuel data diverge systematically from those for unirradiated metal, and appear to have a different (lower) activation energy. The investigators hypothesize small, distributed hydride inclusions as the cause of divergence. Their proposed rate law is:

$$\ln R_{\text{dry}} = 10.258 - \frac{5032.7}{T} \quad (1-1)$$

where R_{dry} is again given in mg/cm²-hr and the activation energy is a round value of 10 cal/g mole.

Figure 1-3:
Variation of Gas Composition With Time
in [McD. Baker, et al., 1966] U-O₂-H₂O Experiments.

x = H₂O o = O₂ • = H₂

Figure 1-4: Uranium Oxidation Rate Law Comparison.

Comparison of Uranium Oxidation Rate Laws, $\text{kg/m}^2/\text{s}$. (A) Solid line (top) Bonding correlation for CVD calculations, 22 times the Pearce Oxygen-Free U-H₂O rate law, evaluated at 8 kPa average H₂O pressure; (B) Dash line (second from top) Pearce Oxygen-Free U-H₂O rate law; (C) Dash-Diamond (middle); PNNL correlation for N reactor fuel in dry air; (D) Dash-Dot (second from bottom); Ritchie moist air below 75% relative humidity; and (E) Circle (bottom); McGillivray U-dry air correlation, nearly identical to Trimble's result. Temperature is in C and rate is in $\text{kg/m}^2/\text{K}$. Note (D) and (E) cross unphysically at 40 C.

Figure 1-5: PNNL Uranium-Air TGA Detail.

Figure 1-6: PNNL Uranium-Air TGA Run 18 and 49b Slopes.

Figure 1-7: Comparison of SNF Oxidation Rate in Dry Air to Literature Data.
[Abrefah, et al., 1998]

Rapid oxidation periods have been attributed by the investigators to the presence of large hydride inclusions in the corroded N-reactor fuel. Since hydride would decompose at the higher temperatures used experimentally, it is expected that at low temperatures the average reaction rate of N-reactor fuel would exceed values from literature data, but at higher temperatures agreement between N-reactor fuel data and literature data should be good.

1.2.3 Ignition Theory

Concerns about the ignition potential of uranium metal and hydride can be addressed using the classical thermal ignition theory with a rate law for oxidation. The ignition condition can be determined from a steady-state heat balance. The ignition condition then is the temperature at which the heat evolved is equal to the heat lost. A transient model is useful for the time to ignition, but not really necessary since we are interested in the "last" stable steady-state. Consider the steady energy balance for a bulk sample of uranium metal undergoing surface oxidation and heat losses due to convection and radiation:

$$h (T - T_{\infty}) + \epsilon \sigma (T^4 - T_{\infty}^4) = \dot{m}_{\text{ox}}''(T) \Delta H \quad (1-2)$$

where h is the convective heat transfer coefficient, σ is the Stefan-Boltzmann constant, ϵ is the total emissivity of the oxidized surface, ΔH is the heat of reaction, $\dot{m}_{\text{ox}}''(T)$ is the oxidation rate per unit area, T is the metal temperature, and T_{∞} is the ambient temperature. Note that the geometric parameters of area and volume cancel out because, for a bulk piece of metal, the chemical reaction area is equal to the heat transfer area. Solution of equation (1-2) provides a uranium metal temperature T for a given ambient temperature. Above some sufficiently high temperature (the ignition temperature) there is no solution. As an example, the ignition temperature is 660 K for the following parameters: $h = 21 \text{ W/m}^2\text{-K}$, $\epsilon = 0.75$, and $\Delta H = 3.4 \times 10^7 \text{ J/Kg O}_2$.

For a thin layer of uranium or uranium hydride powder, the steady energy balance can be written in a similar fashion:

$$\frac{6(1-\phi)L}{d} \dot{m}''_{\text{ox}}(T) \Delta H = h(T - T_{\infty}) + \epsilon \sigma (T^4 - T_{\infty}^4) \quad (1-3)$$

where ϕ and L are the porosity and characteristic dimension of the powder layer, respectively, d is the diameter of the spherical (assumed) particles, T is the powder temperature, and T_{∞} is the ambient temperature. As an example, a thin layer of 2 micron particles would ignite spontaneously at room temperature.

1.2.4 Experimental Basis

Tetenbaum, et al., studied the influence of uranium particle size and uranium powder height on ignition temperature [Tetenbaum, et al., 1962]. Metal powder charges were placed in stainless steel crucibles of varying diameter in the range 6.35-19.05 mm (see Figure 1-8). Powder heights covered the range of 0-16 mm. Plots of the measured uranium powder ignition temperature versus powder depth are shown in Figures 1-9 and 1-10 for particle diameters $d = 60 \mu\text{m}$ and $d = 840 \mu\text{m}$, respectively. Ignition temperature was measured by heating the furnace containing the crucible in oxygen, at a known rate, and recording the temperature of the crucible.

Epstein, et al., explained Figures 1-9 and 1-10 using a two-dimensional cylindrically-symmetric temperature distribution in the powder [Epstein, et al., 1994 and 1996]. Ignition theory for Tetenbaum's experiments considers the limits of a steady condition whereby the chemical heat production within the powder is balanced by heat conduction through the powder to the crucible walls. The basic equation is that for steady-state heat conduction in a finite cylinder with local heat generation at the constant volumetric rate $6(1-\phi)\Delta H \dot{m}''_{\text{ox}}(T)/d$. For an effective powder bed thermal conductivity k_b , this equation has the form:

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} = - \frac{6(1-\phi)\Delta H}{k_b d} \dot{m}''_{\text{ox}}(T) \quad (1-4)$$

where z is the vertical coordinate measured from the bottom of the crucible and r is the radial coordinate measured from the vertical axis of the crucible.

Figure 1-8: Tetenbaum's Experimental Apparatus.

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Figure 1-9: Crucible Wall Ignition Temperature Versus Uranium Powder Height in Different Diameter Crucibles - Ignition Theory Compared With Experimental Data of Tetenbaum, et al., [1962].

Figure 1-10:

Crucible Wall Ignition Temperature Versus Uranium Powder Height
in Different Diameter Crucibles - Ignition Theory Compared
With Experimental Data of Tetenbaum, et al., [1962].

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Without considering the details of the solution of equation (1-4), we note that calculated values agree reasonably well with the experimental values, as shown in Figure 1-9 and 1-10. Epstein's calculated values are shown in these figures under the label of "Theory". After a critical value, theoretical ignition temperature is independent of height. When the bed is shallow, most of the heat is conducted downward to the radius of the crucible. When the bed is thicker, the resistance to downward heat conduction increases and the ignition temperature decreases. If the bed depth keeps increasing, radial heat conduction to the crucible wall becomes dominant. But the radial distance for heat removal remains constant no matter how deep the powder bed, and the ignition temperature becomes independent of the depth.

1.2.5 Application to MCO Analysis

The foregoing discussion demonstrates that reactions of uranium and the potential for pyrophoric behavior can be reliably quantified when appropriate rate laws, heat transfer relationships, and initial conditions (such as exposed surface area) are known. Therefore the temperature gradient across an MCO rubble basket and the individual fuel element temperatures must be included in a model. Also, the damage fraction, or amount of exposed metal surface area, must be estimated and considered as a function of position in the MCO.

1.3 Fission Product Release

1.3.1 Experimental Basis

Fission product releases should be estimated as part of an integrated accident analysis, but due to a paucity of experimental data, there is no fission product release model in HANSF. The existing metal fuel fission product release database consists solely of Hilliard's experiments [Hilliard, et al., 1961]. Hilliard's approach was to heat small specimens of irradiated uranium in a tube and collect the released material from the flowing air stream at the end of the tube. Afterward, the remaining test specimen was dissolved to determine the amount of each fission

product that remained. The initial amount of each material was assumed to be the sum of the collected amount and the amount remaining in the test specimen. The fraction of material released is then simply the ratio of the collected material to the total material. Test samples were bare natural uranium cylinders measuring 1/4 inch in diameter, 3/4 inch long, and weighing 11.5 grams. Specimens were irradiated to 2.4×10^{14} nvt and then allowed to cool for 22 to 70 hours prior to testing.

Hilliard felt that a complete study of fission product release would consider at least six variables: type of fuel, atmosphere, temperature, time of heating, fuel element geometry, and irradiation level. Hilliard's study was limited for the most part, however, to consideration of time of heating and temperature. A summary of experimental conditions is presented here as Table 1-1. Eight fission products were considered: iodine, tellurium, xenon, strontium, cesium, ruthenium, barium, and zirconium.

Hilliard's results indicate that temperature had "a profound effect on the fraction of fission products released." Figure 1-11 illustrates per cent released versus temperature for iodine, tellurium, and xenon. Note that furnace temperature, not fuel temperature, is recorded. All experiment points are based on a 24 minute heating time. Hilliard states that the area near the uranium melting point is probably an inflection, but is uncertain. The effect of temperature on strontium, cesium, ruthenium, and barium was definite, but not as pronounced.

A study of Table 1-1 and Figure 1-11 indicates that for the purpose at hand, Hilliard's data provide only a rough idea of what postulated fission product releases might be for the MCO design. MCO values for Hilliard's six variables do not necessarily match any test conditions noted in Table 1-1. It is also difficult to apply Hilliard's results to an MCO case because of differences between measured furnace temperatures and the actual fuel temperature. For example, the ignition temperature predicted for a solid piece of uranium metal (387°C, or 660 K) falls well below the data in Figure 1-11. Hilliard noted that fuel temperature excursions made it impossible to measure or control fuel temperature, which could be about 500°C higher than the furnace temperature.

Figure 1-11: Effect of Temperature on Release of Iodine, Tellurium, and Xenon.

Table 1-1: Summary of Hilliard's Experimental Conditions

Run No.	Furnace Temp. (°C)	Time (min.)	Air Velocity (cm/min)	Remarks
A-1	1200	10	500	*
A-2	1210	10	500	*
A-3	1215	50	500	*
A-6	1215	25	500	
A-7	1215	44	500	
A-8	1215	51	500	
A-9	1215	86	500	
A-10	1215	2.5	500	
A-11	1215	85	500	
A-12	1215	48	500	
A-13	1440	24	500	
A-14	990	24	500	
A-15	620	24	500	
A-16	1215	26	500	
A-17	1215	25	25	Air flow 1/20th normal.
A-18	1215	24	500	
A-19	30-1325	150	500	Furnace programmed for 10°C/min rise.
A-20	1440	11	500	
A-21	620	99	500	
A-22	1220	10.5	500	
A-23	1215	120	500	
A-24	990	50	500	
A-25	425	232	500	
A-26	1215	84	500	40 min. in Air, then 44 min. in Helium.
A-27	535	115	500	
A-30	70-1030	80	500	Furnace programmed for 10°C/min rise.
A-31	70-1170	110	500	Furnace programmed for 10°C/min rise.
H-1	1215	25	500	Helium atmosphere.
* In the first three runs, the specimen was brought up to temperature and cooled in helium atmosphere. In all other runs, air flowed over the specimen during the entire run.				

1.3.2 Application to MCO Analysis

There are unfortunately at present no correlations that may be used for fission product release from fuel in an MCO. NRC correlations in standard use for commercial oxide fuels do not apply to metal fuel. Follow-up work at Hanford after Hilliard is sparse. Possible courses of action are:

1. Model Hilliard's experiments to deduce appropriate fuel temperatures and oxidation rates. These are absolutely required to interpret (correlate) the data.
2. Given step 1 above, compare Hilliard's data to correlations for oxide fuel and judge the efficiency of modifying the correlations.
3. Create a correlation given knowledge of the oxidation rate and oxygen potential of the U-Pu-O system, and transport properties.
4. Seek declassification of pertinent data as may exist.

1.4 Uranium Oxide Hydrate Decomposition

1.4.1 Unirradiated Material Data

Corroded fuel placed in an MCO is expected to contain oxide present either as a layer adherent to metal surfaces, or as particulate somehow remaining attached to or within fuel elements and scrap. The oxide, also referred to as "sludge", is expected to have some chemically bound water in the form of hydrates. Because thermal decomposition releases hydrate water and makes it available for uranium oxidation, hydrate decomposition models are needed as part of integral MCO assessment. A quantitative assay of the hydrates is not complete, and a bounding assessment requires that all sludge consists of $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ and $\text{UO}_4 \cdot 4\text{H}_2\text{O}$. Only $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ thermal decomposition is considered in HANSF, due to the lack of thermal decomposition data for UO_4 hydrates.

Danroc obtained data for decomposition of unirradiated $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ for very low pressure, 10^{-5} torr (about 1.3×10^{-3}), first at 25°C , and then during a linear temperature increase, as shown in Figure 1-12 [Danroc, 1982]. The abscissa is percent weight loss, while the first part of the ordinate shows the time at ambient temperature, and the second part of the ordinate shows temperature. A family of curves is denoted by "D =" which is the number of days that the uranium fuel was treated in air at 80°C and 80% relative humidity. Drying data show that for ambient conditions, decomposition from $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ to $\text{UO}_3 \cdot \text{H}_2\text{O}$ takes place in less than four hours; this corresponds to half the total weight loss. Further weight loss is obtained only by increasing the temperature. Drying data show that the hydrate decomposes from $\text{UO}_3 \cdot \text{H}_2\text{O}$ to $\text{UO}_3 \cdot x\text{H}_2\text{O}$, where x is in the range of 0.8 to 0.9, between about 80°C and 160°C . The data also demonstrate that complete drying to $x=0$ is difficult even under high vacuum, except at very high process temperatures of about 300°C .

1.4.2 K-Basins Sludge Water Content and Dehydration Characterization Data

K-basins spent fuel characterization data from [Abrefah, et al., 1997a and 1997b], comprised of seven runs (TGA #40 through #46), are considered here.

Sample heatup and dwell schedules were as follows:

- a. Ramp of $1^\circ\text{C}/\text{min}$ to 50°C , 8 hour dwell,
- b. Ramp of $1^\circ\text{C}/\text{min}$ to 75°C , 10 hour dwell,
- c. Ramp of $1^\circ\text{C}/\text{min}$ to 300°C (TGA #40 through #42) or $0.2^\circ\text{C}/\text{min}$ to 300°C (TGA #43 through #47), 12 hour dwell,
- d. Ramp of $1^\circ\text{C}/\text{min}$ to 425°C , 12 hour dwell, and
- e. Ramp of $2^\circ\text{C}/\text{min}$ to 625°C , 6 hour dwell.

It is reasonable to assume that: (1) weight loss during the 50°C dwell is mostly free pore water evaporation, (2) weight loss during the 625°C phase is mostly oxygen loss [Wheeler, et al.,

Figure 1-12: $\text{UO}_3 \cdot \text{H}_2\text{O}$ Drying Curve [Danroc, 1982].

1964], and (3) dehydration primarily occurs in phases b, c, and d of the experiments. Abrefah, et al., take this view too. However, it is also possible that some weight loss at 75°C is from free pore water, and that both water and oxygen are lost during the ramp to 625°C.

Table 1-2 summarizes weight loss in each phase of the PNNL experiments. Under the assumptions that (a) All weight lost at and below 50°C is free water, and (b) All weight lost above 425°C is oxygen, values in Table 1-3 are derived for the water weight percent with respect to the initial mass of hydrated sample. The exceptional case for the derivation is that of TGA #46, because this experiment was performed at atmospheric pressure, so that even water evolved at 75°C must contain free water. Hence, the weight loss from TGA #44, also from sample ID 96-08, was used for the initial weight loss of TGA #46 after adjustment by the ratio of post-test sample weights.

Water content in Table 1-3 is consistently derived with respect to the way the water fraction of a hydrate would be calculated, i.e., before water loss. Thus if a sample contained only $\text{UO}_3 \cdot 2\text{H}_2\text{O}$, its maximum total weight loss would be 11.1%. The data show that sludge samples were generally only partially hydrated, but one exceptional case exists for TGA #45 which remains unexplained. The average weight fraction, including this sample, is 7.1% water.

Recently, [Abrefah, Buchanan, and Marschman, 1997] presented Arrhenius rate law parameters for individual TGA experiments. These were analyzed by [Plys, 1997] to arrived at the following best-fit parameters for an equation of the form $k = k_0 e^{-Q/T}$:

Step	Pre-Exponential Factor, inverse minutes	Activation Energy, Kelvins
1. $\text{UO}_3 \cdot 2\text{H}_2\text{O} \rightarrow \text{UO}_3 \cdot \text{H}_2\text{O}$	980	5111
2. $\text{UO}_3 \cdot \text{H}_2\text{O} \rightarrow \text{UO}_3 \cdot 0.5\text{H}_2\text{O}$	34280	7241
3. $\text{UO}_3 \cdot 0.5\text{H}_2\text{O} \rightarrow \text{UO}_3$	6161	7548

Date: 12/31/98

1 - 24

FAI/98-40, Rev. 1

Table 1-2: Drying Results of the Last Seven KE Canister Sludge Samples [Abrefah, et al., 1997a & 1997b]									
Sample		Sample Weight Loss (mg) for Different Temperature Ranges							
		Weight (mg)	RM to 50°C	Held at 50°C	50°C to 75°C	Held at 75°C	75°C to 300°C	Held at 300°C	300°C to 425°C
TGA Run #	ID								Held at 425°C
40	96-13	1159	0.67	1.70	0.18	3.13	20.83	7.25	1.55
41	96-13	768	0.23	1.04	0.25	2.10	11.80	2.75	0.64
42	96-15	723	0.65	3.33	0.64	6.05	22.18	4.56	1.93
43	96-15	1108	NE	NE	1.52	0.65	33.39	3.84	0.53
44	96-08	1004	0.94	1.23	0.01	2.16	28.02	2.52	2.31
45	96-04/L	471	0.32	2.66	1.60	9.24	44.70	4.10	4.63
46	96-08	771	9.87	49.84	1.55	9.56	28.31	3.18	2.18
									2.62
									1.22
									1.17
									1.49
									0.73
									2.16
									1.49
									2.42
									1.76
									1.22
									1.17

Table 1-3: Interpreted Canister Sludge Dryout Results					
TGA Run #	Weight After Test (mg)	Weight After 425°C Dwell	Weight After Ramp to 75°C	Weight Loss 50°C to 425°C	% Weight Assumed Hydrate
40	986	989.04	1022.91	33.87	13.0%
41	654	655.08	673.16	18.08	2.7%
42	603	604.64	640.78	36.14	5.6%
43	984	986.0	1027.93	41.93	4.1%
44	322	324.89	361.40	36.51	10.1%
45	358	361.25	427.94	66.69	15.6%
46	440	442.49	481.75 (1)	39.26 (1)	8.1% (1)

(1) Use TGA #44 data at 75°C times sample weight ratio to correct for free water, or 2.97 g lost through 75°C.

1.4.3 Application to MCO Analysis

Unfortunately at present, there are no quantitative data regarding the amount of hydrate that can be present in fuel sludge, or its stoichiometry. There is also a paucity of $\text{UO}_4 \cdot x\text{H}_2\text{O}$ data, but the $\text{UO}_3 \cdot x\text{H}_2\text{O}$ data are sufficient for model development. In summary, important aspects of hydrates for MCO analysis are:

1. Quantity and stoichiometry, which are as stated not a priori known.
2. Equilibrium decomposition data, which are known for $\text{UO}_3 \cdot x\text{H}_2\text{O}$.
3. Kinetic rate law data to provide the decomposition rate as a function of temperature and pressure.

The presently available data allow only a rough interpretation of rate limitations.

1.5 Aerosol Transport and Deposition

1.5.1 Experimental Basis

The final step in the integrated accident analysis involves aerosol transport and deposition. The experimental and modeling basis for aerosol behavior is mature and techniques used for nuclear reactor safety may be readily applied here. In this section we simply note that a correlation based approach is used for coagulation and sedimentation, subject to two assumptions:

1. All aerosol particles are regarded as having the same chemical composition due to the rapidity of coagulation versus settling.
2. The aerosol size distribution is assumed to conform to one of two universal, source-independent dimensionless distributions, one for an aerosol in equilibrium with its source and one for a decaying aerosol with a negligible source.

This approach has been validated against the well-known AB-5 experiment performed at Hanford [Hilliard, et al., 1983]. AB-5 was performed in the Containment Systems Test Facility (CSTF), which, as shown in Figure 1-13, is an 850 m³ (30,000 ft³) carbon steel vessel with a design pressure of 0.517 MPa (75 psig). For roughly 900 seconds, a spray system pumped sodium aerosol at 563°C into the CSTF at a rate of 445 g/s. The CSTF remained sealed for 8,560 minutes. During the test, suspended mass concentration, particle size distribution, and chemical composition were measured by passing a known quantity of gas through small filters. Figure 1-13 shows suspended aerosol mass concentration as a function of time.

1.5.2 Application to MCO Analyses

Aerosol transport and deposition are important to the scope of the HANSF tool and an approach adopted for nuclear reactor severe accident analysis is adopted here [Epstein and Ellison, 1988]. The approach, described in Section 2.4, accounts for time-dependent aerosol sources, leakage through junctions, and removal mechanisms such as impaction and sedimentation, and tracks suspended aerosol mass and deposited mass in each compartment.

1.6 Counter-Current Flow

1.6.1 Experimental Basis

Gas flow between compartments can be uni-directional when the pressure difference is large, or it can be counter-current when the pressure difference is small or zero, but there is a density difference. If the pressure-driven unidirectional flow is large enough, counter-current flow does not take place, and the forced flow is said to "flood" or purge the flowpath. If the pressure-driven flow is below the flooding limit, counter-current flow accounts for some or all of the aerosol and gas transport. Density-driven counter-current flow can be dominant after an initial pressure transient. In general, counter-current volumetric flowrate Q_{cc} depends on the

Figure 1-13:
Containment Systems Test Facility for Test AB-5 and Test Results
for Suspended Mass [Hilliard, et al., 1983].

density difference, the flow orientation (vertical or horizontal), and the length-to-diameter ratio L/D of the flowpath.

For simple geometries, namely horizontal junctions in floors and ceilings and vertical junctions in walls, the correlations of Epstein [Epstein, 1988] can be used to determine both the counter-current flowrate and the flooding flow. These correlations are based on sets of brine-water experiments that take advantage of the fact that salty water is denser than fresh water. Results from this simple arrangement are valid for other situations where molecular viscosity and thermal diffusivity are not important; i.e., purely density-driven flow. Epstein has confirmed that the correlations are applicable to gases by comparing correlation results to experimental data derived from gas flows. As an example, experimental results and asymptotic physical model predictions for a horizontal junction (vertical flow) are shown in Figure 1-14. A single correlation was developed by Epstein to cover the entire data range, and is used for practical application. The parameter range for which the correlation is valid based on experimental evidence is:

$$0.01 < L/D < 20 \quad \text{and} \quad 0.025 < \Delta\rho/\bar{\rho} < 0.17 \quad (1-5)$$

but the correlation should be valid to higher values of $\Delta\rho/\bar{\rho}$.

1.6.2 Application to MCO Analysis

Counter-current flow can be an important mechanism in MCO accident scenarios. Postulated MCO accident scenarios typically involve an initial pressurization phase in the MCO or canister storage building. After this initial phase, gas and aerosol transport could continue due to counter-current exchange. HANSF accounts for these phenomena using Epstein's experimental correlations.

Figure 1-14: Pure Counter-Current Flow Through a Rectangular Flowpath in a Horizontal Wall, i.e., Vertical Flow [Epstein, 1988].

1.7 Nitriding

1.7.1 Experimental Basis

Nitriding is the reaction of uranium fuel with nitriding agent, namely, nitrogen gas in this instance. Various compounds can be formed: UN, U_2N_3 , and $UN_{1.75}$. Mallett and Gerds studied the surface reactions of a very pure uranium billet with nitrogen at a pressure of 1 atm, with a temperature range between 550 and 900°C [Mallett and Gerds, 1955]. Their results can be summarized as follows:

1. Nitrogen reacts with uranium parabolically in the temperature range studied.
2. Below 750°C, reaction products consist primarily of UN_2 . (This conclusion is contradicted by [Katz, et al., 1986], as discussed below.)
3. Between 775 and 900°C, reaction products consist of UN, UN_2 , and U_2N_3 .

Mallett and Gerds express the kinetics according to a parabolic rate law,

$$\frac{dW^2}{dt} = k(T) \quad (1-6)$$

where W is the nitrogen consumed (ml/cm^2) and k is the temperature-dependent rate constant (ml/cm^2)²/s; the volume of nitrogen consumed was measured at standard temperature and pressure. Mallett and Gerds derived rate constants for two temperature ranges. For the range from 550 to 750°C,

$$k = 202 \exp(-25,500/RT) \quad (ml/cm^2)^2/s \quad (1-7a)$$

and for the range from 775 to 900°C,

$$k = 3.95 \exp(-15,100/RT) \quad (ml/cm^2)^2/s \quad (1-7b)$$

where T is the temperature in K, and R is the gas constant (cal/mole-K).

Katz, et al., state the UN₂ formerly believed to exist cannot be prepared under ordinary conditions [Katz, et al., 1986]. Nitrides can be prepared from the reaction of very pure uranium metal (or dehydrided uranium hydride) with very pure nitriding agents. To prepare nitrides, the metal surface must be free of even trace quantities of oxide or oil films.

Given Katz's discussion, nitriding is secondary, relative to decay heat and/or the chemical heat of oxidation. This can be demonstrated by comparing the heat generation from nitriding with heat generation from oxidation. Now the heat of reaction for oxidation of uranium with pure oxygen is 3.4×10^7 J/kg O₂, and the heat of formation of U₂N₃ is 736 KJ/mol, or 2.6×10^7 J/kg N₂. Therefore, we only need to compare the rates of oxygen and nitrogen consumption at a given temperature. Use the Mallett and Gerds rate constants for nitriding and the Pearce oxidation correlation for "dry" conditions at temperatures above 300°C (see Table 3-2):

$$\frac{dW}{dt} = \frac{0.01}{3600} \times 10^{(28.381 - 7 \log T - 4638.2/T)} \quad (\text{kg/m}^2\text{-s}) \quad (1-8)$$

where T is temperature in K. Considering the first one-second interval of the respective reactions and a range of temperatures, oxygen consumption (in kg/m²-s) is an order of magnitude larger than nitrogen consumption. For example, at 700°C nitriding proceeds at 1.0×10^{-4} kg/m²-s, while oxidation in pure oxygen proceeds at 1.0×10^{-3} kg/m²-s. Moreover, the nitriding reaction rate decreases over time, due to the parabolic rate law kinetics.

1.7.2 Application to MCO Analysis

Conclusions drawn here are similar to those drawn in Section 1.2.4 for uranium oxidation: behavior can be quantified when appropriate rate laws, heat transfer relationships, and initial conditions such as exposed surface area are known. Inclusion of nitriding in MCO analysis is undoubtedly conservative. Nitriding has only been observed with very clean uranium and pure nitrogen -- conditions that are unlikely to exist in the MCO.

1.8 Copper Corrosion

1.8.1 Experimental Basis

Scrap basket designs contain copper because of its heat transfer properties. Here we consider the potential for copper corrosion in the MCO. Copper has excellent corrosion resistance in steam and nitrogen atmospheres, and exhibits scaling in oxygen at high temperatures [CDA, 1997]. Experimental data for copper corrosion in pure nitrogen and steam are sparse, but owing to the many industrial applications, data for corrosion in water and air are abundant. There is a fair amount of data for oxidation in pure oxygen.

Because [CDA, 1997] suggests oxidation at high temperatures, consider the reaction rate for

JANAF Thermochemical Tables report that the heat of formation, Q_r , of Cu_2O is 170.71 kJ/mol. This converts to 5.3×10^6 J/kg O_2 , which compares to 3.4×10^7 J/kg O_2 for the oxidation of uranium by oxygen.

At or above 900°C, the reaction of copper and oxygen follows a parabolic rate law [Li and Lo, 1965; and Roy, et al., 1991]:

$$W^2 = k(T)t \quad (1-9)$$

where W is mass gain per unit area (kg/m^2) and k is the temperature-dependent rate constant (kg/m^2)²/s. The rate constant is weakly dependent on oxygen partial pressure [Roy, et al., 1991]:

$$\frac{k_1}{k_2} = \left(\frac{P_1}{P_2} \right)^{\frac{1}{7}} \quad (1-10)$$

The reaction constant is then 25% higher at 1 atm than at 0.21 atm.

Li and Lo studied the oxidation of copper in the temperature range between 200 and 900°C under a pressure of 76 mm Hg. Results show that the reaction obeys a cubic law between 200 to 350°C, and a parabolic law between 600 and 900°C. Between 400 and 550°C, the reaction is initially parabolic. Li and Lo report that at 400°C, $W = 200$ micro-grams/cm² at 200 minutes, which leads to $k = 3.3 \times 10^{-10}$ (kg/m²)²/s.

Compare the reaction rate for copper oxidation in oxygen with that for uranium oxidation in oxygen, using conditions of 400°C and 1 atm of oxygen. We have already calculated $k = 3.3 \times 10^{-10}$ (kg/m²)²/s for 400°C and 76 mm Hg. Correcting for 1 atm using equation (1-8) gives $k = 4.6 \times 10^{-10}$ (kg/m²)²/s. At, say, $t = 1$ second, the copper oxygen consumption rate at 400°C and 1 atm oxygen is 2.1×10^{-5} kg/m²-s. The Pearce rate law at 400°C gives an oxygen consumption rate of 1.4×10^{-4} kg/m²-s. The mass gain of oxygen by copper is comparable to that by uranium for a fraction of a second, but becomes negligible after a few hundred seconds.

1.8.2 MCO Application

In light of the measured reaction rates in oxygen, there are no copper corrosion models in the HANSF code. Relative to oxidation, hydriding, and nitriding, copper corrosion is unimportant.

1.9 Uranium Hydrides

Uranium hydrides (UH₃) are produced as fine particles that provide a large surface area for an exothermic chemical reaction. The uranium hydride reacts with oxygen and the dehydrided uranium hydride reacts with both oxygen and water vapor with essentially the same heat of reaction as uranium metal oxidation. The highly reactive surface (because of a large

area-to-volume ratio) becomes benign only when the fine particles turn into the stable oxide. Another practical implication of uranium hydride is that it can be a source of hydrogen gas as it decomposes into finely divided uranium metal. Such finely divided uranium metal can also be rehydrided under a high hydrogen partial pressure.

Hydride formation or decomposition is represented by the reaction:

The direction of the reaction depends on the hydrogen pressure relative to equilibrium. If the hydrogen pressure is above equilibrium, hydriding occurs; if the hydrogen pressure is below equilibrium, dehydriding occurs. Equilibrium pressure of H_2 over UH_3 at about 430°C is one atmosphere. An equation for decomposition hydrogen pressure, P_D , in mm of Hg is:

$$\log P_D = 9.28 - \frac{4500}{T} \quad (1-11)$$

where T is in degrees K. This is illustrated in Figure 1-15, from which it can be seen that UH_3 is thermally stable during interim storage with only a slight pressure of hydrogen present, less than 1 mm Hg. The impact of this equilibrium relationship is shown in Figure 1-16, where a maximum in the hydriding rate occurs at a temperature below the equilibrium value, and the rate is of course zero at equilibrium.

Hydrides are formed naturally as a small fraction of uranium metal corrosion product under water. [McD Baker, et al., 1966] showed a range of 2 - 8% hydride based on a defect in measured hydrogen generation. We do not a priori know the distribution of hydride between the oxide and metal for N reactor fuel.

Figure 1-15: Decomposition Pressure vs. Temperature for UH_3 [Kitzes, 1950].

Figure 1-16:

The Temperature Dependence of the Reaction Front Velocity U
for Two Working Pressures, 3.5×10^6 and 6.6×10^4 Pa:

_____, Regions which fit an Arrhenius relation [Bloch and Mintz, 1981].

1.9.1 MCO Application

Formation and/or decomposition of uranium hydride can be predicted with appropriate rate laws if surface temperature and hydrogen partial pressure are known. This is a necessary part of integrated accident analysis, owing to the highly reactive nature of dehydrated uranium hydride.

1.10 Natural Circulation Inside the MCO

1.10.1 Experimental Basis

Global natural circulation refers to the natural convection flows that develop in the (sealed) MCO due to local temperature differences. Global natural circulation within the MCO should be distinguished from counter-current flow. Counter-current flow occurs in junctions connecting compartments with different gas densities. Here we consider the potential for global natural circulation within the MCO. In particular, we evaluate how much global circulation enhances heat transfer, vis-a-vis pure conduction.

Local convection may be evaluated by considering natural circulation in a narrow vertical enclosure, such as between fuel assemblies or within a fuel assembly annulus. Gebhart, et al., [1988] summarize studies of transport in such tall enclosures. The average convective transport is often expressed as a function of the Rayleigh number

$$Ra = \frac{g\beta d^3 \Delta T}{\alpha_f \nu_f} \quad (1-12)$$

and the aspect ratio

$$A_r = \frac{L}{d} \quad (1-13)$$

- where d = the distance between the vertical walls, taken here to be the hydraulic diameter d_H (0.025 m),
 L = the enclosure height (0.66 m),
 ΔT = the temperature difference between the walls (10°C),
 β = the expansion coefficient (0.003 1/K),
 α_f = the gas thermal diffusivity (3×10^{-5} m²/s), and
 ν_f = the gas kinematic viscosity (2.1×10^{-5} m²/s).

Property values are those for nitrogen at 350 K. Using the parameter values listed above leads to $A_r = 26$ and $Ra = 7000$.

For the convection dominated regime in a vertical cavity, the overall Nusselt number [Gebhart, et al., 1988] is

$$Nu = 0.365 \left(\frac{Ra}{A_r} \right)^{1/4} \quad (1-14)$$

which yields $Nu = 1.5$ for the present example conditions. This represents a modest enhancement over pure conduction ($Nu = 1$) and is a rather weak function of ΔT . Local natural circulation heat transfer is therefore expected to play a relatively minor role in MCO cooling.

Figure 1-17 shows predicted values of Nu for natural convection in a vertical annular porous layer. The modified Rayleigh number is:

$$Ra' = \frac{g L \beta \Delta T K}{\nu_f \alpha_f} \quad (1-15)$$

where K is the permeability of the porous layer. Figure 1-17 shows that for large aspect ratios, Nu is not much larger than 1.0, which indicates global circulation does not greatly augment pure conduction.

Figure 1-17: Nusselt Number for Natural Circulation in an Annular Porous Layer.

1.10.2 Application to MCO Analysis

Because global natural circulation is not expected to greatly enhance heat transfer, it is not included in HANSF MCO models. Heat transfer occurs directly between heat sinks, as discussed in Section 3.6.2, with a small amount of heat diverted so that gas pockets assume a mean temperature based on adjacent heat sink temperatures.

1.11 Reactive Area Distribution

A key question for modeling fuel elements in an MCO is whether or not an uneven distribution of reaction area can lead to a significant non-uniform axial temperature profile. For example, because fuel elements tend to be damaged at ends, the reactive area may be located primarily there instead of uniformly distributed in a basket. Depending upon the reaction power, fuel thermal conductivity may be large enough to quickly conduct heat away from the reaction area. Otherwise, a temperature gradient must be considered.

1.11.1 Fuel Element Axial Temperature Profile

A general procedure for examining the validity of a spatially uniform temperature assumption is to write a complete energy balance for the fuel element, one that includes axial heat conduction, and then evaluate the temperature difference between the reacting end of the element and the protected, nonreactive opposite end of the element. The following simplifying assumptions are made:

- (1) The aspect ratio of the fuel element is large enough so that heat conduction is virtually one-dimensional and in the axial z-direction.
- (2) The physical properties of the fuel-element material are constant.

- (3) Surface oxidation occurs at one end of the fuel element and over an axial length z_0 that is small compared with the total length L of the element.
- (4) The surface-oxidation heating rate is converted into an effective axial heat flux $\dot{q}''$ that impinges upon the reactive, axial end of the element located at the position $z = 0$.
- (5) The opposite, nonreactive end of the element at $z = L$ is taken to be an adiabatic surface.
- (6) The fuel element loses heat (laterally) to adjacent fuel elements or the MCO wall at a rate that follows Newton's law of cooling.

With the foregoing assumptions, the governing equation describing the axial temperature field $T(z,t)$ within the fuel element is

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} + \dot{Q}'' - ah[T - T_\infty(t)] \quad (1-16)$$

where k , ρ , c , are, respectively, the thermal conductivity, density, and specific heat of the fuel element, t is time, $\dot{Q}''$ is the volumetric decay heat generation rate, "a" is the side surface area-to-volume ratio of the fuel element, and h is the coefficient of heat transfer from the fuel element of interest to an adjacent fuel element (or MCO wall) with a known temperature history $T_\infty(t)$. Note that in accord with Assumption (6), h is assumed constant, but nevertheless capable of representing the combined effects of lateral heat removal by radiation, conduction and/or natural convection. The initial and boundary conditions are:

$$T = T_0 \quad \text{at} \quad t = 0 \quad (1-17)$$

$$-k \frac{\partial T}{\partial z} = \dot{q}'' \quad \text{at} \quad z = 0 \quad (1-18)$$

$$\frac{\partial T}{\partial z} = 0 \quad \text{at} \quad z = L \quad (1-19)$$

Boundary conditions of equations (1-18) and (1-19) follow from Assumptions (4) and (5). Note that the effective surface-reaction flux in equation (1-18) is related to the actual surface oxidation flux $\dot{m}_{ox}$ (in kg O₂ m⁻² s⁻¹) by

$$\dot{q}'' = z_0 a \Delta H \dot{m}_{ox} \quad (1-20)$$

where ΔH is the heat of reaction (in J/kg O₂). Recall that z_0 is the axial length over which the surface reaction takes place ($z_0 < L$).

The sought temperature difference is

$$\Delta T = T(0,t) - T(L,t) = \frac{\dot{q}''}{kb} \left[\frac{\cosh(bL) - 1}{\sinh(bL)} \right] \quad (1-21)$$

$$\text{where } b = \left(\frac{ah}{k} \right)^{1/2} \quad (1-21a)$$

To employ equation (1-21) directly, the temperatures for evaluation of q'' and h must be known. The heat source should be evaluated at $T(0, t)$, while h should be evaluated at an intermediate temperature, or conservatively at $T(L, t)$. The heat source is evaluated by a Taylor series expansion of the Pearce oxygen-free water vapor reaction rate law which may be written as

$$\dot{m}_{ox} = C p^{1/2} e^{-T_E/T} \quad (1-22)$$

where $C = 5.939 \times 10^{-2}$ kg/m² s,

$T_E = 4936.7$ K, and

$p =$ steam partial pressure, kPa.

$$e^{-T_E/T} \approx e^{-T_E/T_r} e^{T_r \theta} \quad (1-23)$$

$$T_r = \frac{T_E}{T(L, t)} \quad (1-24)$$

$$\theta = \frac{T - T(L, t)}{T(L, t)} \quad (1-25)$$

So, the heat source becomes

$$q'' = z_o a \Delta H C p^{1/2} e^{-T_r} e^{T_r \theta} \quad (1-26)$$

and substituting into equation (1-21) yields

$$T_r \theta_o e^{-T_r \theta_o + 1} = B \quad (1-27)$$

$$\theta_o = \frac{T(0, t) - T(L, t)}{T(L, t)} \equiv \frac{T_o - T_L}{T_L} \quad (1-28)$$

$$B = \frac{z_o a \Delta H C p^{1/2} T_r}{k b T_L \exp(T_r - 1)} \frac{\cosh(bL) - 1}{\sinh(bL)} \quad (1-29)$$

To further simplify the evaluation, note that if decay power is much greater than axially conducted reaction power at the end $x = L$, then in the steady-state

$$T(L, t) - T_\infty = \frac{Q'''}{h\alpha} \quad (1-30)$$

where α is the value of "a" reduced to account for heat loss over less than 100% of the perimeter. The same substitution is made when calculating "b" in equation (1-21), but not when evaluating the heat flux in equations (1-26) and (1-29). Defining the gas conduction and linearized radiation heat transfer coefficients,

$$h = h_{\text{rad}} + h_{\text{con}} \quad (1-31)$$

$$h_{\text{rad}} = 4\bar{\epsilon} \sigma T(L, t)^3 \quad (1-32)$$

$$\bar{\epsilon} = \left(\frac{2}{\epsilon} - 1 \right)^{-1} \quad (1-33)$$

$$h_{\text{con}} = \frac{k_g}{\delta} \quad (1-34)$$

The steady-state end temperature is given implicitly by

$$T_L = T_\infty + \frac{Q''' / \alpha}{k_g / \delta + 4 \sigma \epsilon T_L^3} \quad (1-35)$$

Calculations of the axial element temperature difference are performed with values listed in Table 1-4. The fuel element surface for heat loss is a fraction of its total because neighbor elements are either identical or at higher temperature, so a factor of 33% is chosen to multiply "a". Table 1-4 also contains a single set of derived values as an example.

Figure 1-18 illustrates the axial temperature difference along a fuel element for various ambient steam pressures and effective rate law enhancement factors, as a function of the effective ambient heat rejection temperature. Note the heat rejection temperature varies over a range including low values when neighbor elements cool down during evaporation, and high values when neighbor elements heat up after basket dryout. The damaged element in question is dry because no credit is taken for evaporative heat removal, but it is supplied with steam from wet elements in a lower basket. It is typical during cold vacuum drying for the steam pressure to initially be near 12 kPa, saturation at 50°C, but thereafter to decrease to values in the range of 1 to 4 kPa. This is because evaporative cooling lowers the local temperature and hence the saturation pressure; 4 kPa is the saturation value at about 30°C and element temperatures can decrease to 10°C or lower. Rate enhancement factors chosen in Figure 1-18 represent surface area increases due to roughness, cracking, or hydrides (which have high specific area).

It is seen from Figure 1-18 that the influences of steam partial pressure and rate enhancement become increasingly important for temperatures above 50°C. Further, for heat rejection temperatures greater than 75°C and a combination of high steam partial pressures and rate law enhancement factors, the axial temperature difference increases rapidly and thermal stability becomes an issue. But for steam pressures corresponding to long-term behavior during CVD, near 4 kPa, or for rate law enhancement factors below 10, the axial temperature

Table 1-4: Calculation of Axial Temperature Difference**A. Input Values**

Reacting Element Length	z_o	0.1 m
Non-Reacting Element Length	L	0.56 m
Surface-to-Volume Ratio	a	220 m ⁻¹
Perimeter Fraction for Heat Loss	-	33%
Thermal Conductivity	k	30 W/m·K
Surface Emissivity	ϵ	0.7
Stefan-Boltzmann Constant	σ	5.67 x 10 ⁻⁸
Maximum Steam Pressure	p	12 kPa
Steam Thermal Conductivity	k_g	0.023 W/m
Gap Between Fuel Elements	δ	0.012 m
Heat of Reaction	ΔH	1.67 x 10 ⁷ J/kg O ₂
Rate Enhancement Factor	F	10

B. Derived Values

Overall Emissivity	$\bar{\epsilon}$	0.5
Radiation Heat Transfer Coefficient (70°C)	h_{rad}	4.6 W/m ² ·K
Conduction Heat Transfer Coefficient	h_{con}	2.0 W/m ² ·K
Fin Parameter	b	3.5 m ⁻¹
Oxidation Rate at 70°C	m''_{ox}	10 ⁻⁷ kg/m ² ·s
Axial Heat Flux	q''	35.1 W/m ²
Temperature Differences for 70°C ambient, F=10	ΔT	4°C

Figure 1-18:

Axial Temperature Difference as a Function of Ambient Temperature for Heat Rejection, for Various Rate Enhancement Factors vs. Literature Data to Represent Surface Area Increases Due to Roughness, Cracking, or Hydrides, and for Various Steam Partial Pressures.

difference lies below 6°C and there is thermal stability, when the heat rejection temperature is up to 75°C.

The preceding results suggest that a combination of high ambient heat rejection temperature, high steam partial pressure, and high reaction rate enhancement factor can lead to large and potentially unstable fuel element axial temperature gradients. Examination of the equations for the axial temperature difference, (1-27) to (1-29), reveals that the dimensionless axial temperature difference θ reaches a maximum when it is equal to $1 / T_r$, and the parameter group $B = 1$. This represents the last stable steady solution for the reacting end temperature T_o , and the criterion $B = 1$ is the ignition criterion. Note that B contains all the input information on the kinetic rate law, system geometry, and boundary conditions, hence the ignition criterion can be used to study parametric tradeoffs between these input values.

Figure 1-19 illustrates the required rate law enhancement for ignition for various steam pressures as a function of the heat rejection temperature. In accord with expectation from Figure 1-18, there is no stable solution for an ambient temperature of about 78°C for the case of high steam pressure, $p = 12$ kPa, and a rate enhancement factor of 22. But for a steam pressure of $p = 4$ kPa, there is thermal stability for a rate law enhancement of 40 given a heat rejection temperature of 75°C.

From Figure 1-19, it is clear that steam pressure and the effective heat rejection temperature at CVD are important contributors to runaway reaction potential, or conversely to margin against runaway. An unusual circumstance, the combination of persistent high steam partial pressure in gas entering the bottom of a dry fuel basket containing badly damaged yet somehow dried out fuel elements, is required for thermal instability.

1.11.2 Application to MCO Analysis

It is concluded that for reasonable enhancements to the nominal (literature) reaction rate that may characterize oxidation of N reactor fuel, for reasonable damage fractions of a fuel

Figure 1-19:

Marginal Rate Law Enhancement Factor (vs. Pearce oxygen-free water vapor) as Function of Ambient Temperature for Heat Rejection, for Various Steam Partial Pressures in kPa. This rate enhancement factor represents extra surface area due to roughness, cracking, or hydrides; the marginal value is a boundary between stable and unstable case.

element, and reasonable variation in steam partial pressure during CVD, the undamaged section can effectively reject reaction power and keep fuel relatively axially isothermal. However, for persistent high steam partial pressures above 8 kPa, for significant rate law enhancements in degraded fuel (> 20 times literature), and for a high heat rejection temperature typical of a fuel basket interior, large axial temperature gradients ($> 10^{\circ}\text{C}$) can exist and there is a potential for thermal instability.

The ability to consider axial variation in fuel element temperature has been included as part of the HANSF code, in light of the discussion above. Ignoring axial variation is often a reasonable assumption, but we expect instances where the added effort of axial nodalization is warranted.

2.0 REGION AND TRANSPORT MODELS

Code description can be divided into two parts: (1) generic region and transport models, and (2) MCO-specific models. Region and transport models are described first.

2.1 Model Structure

A "region" could be the MCO free gas space, the annulus between an MCO and vault tube, or an operating deck space. The region model is designed as a classical state-space representation with mass and energy as state variables and all other quantities such as temperature, pressure, and physical properties as auxiliary variables - an approach consistent with conservation of mass and energy. Thus, the mass of substance i in region r is a state variable described by the explicit differential equation

$$\frac{dm_{ir}}{dt} = \sum W_{ijr} + S_{ir} + \sum W_{ipr} \quad (2-1)$$

where m_{ir} = Mass of compound i region r ,

W_{ijr} = Flow rate of compound i from j to r ,

S_{ir} = Source of compound i in r , and

W_{ipr} = Flow rate of compound i within region r due to process p .

The total energy is described by

$$\frac{dU_r}{dt} = \sum W_{ijr} h_{ijr} + \sum S_{ir} h_r + \sum W_{ipr} h_p \quad (2-2)$$

where h is the enthalpy of the compound and the subscripts are defined above. While these equations are mere bookkeeping, more important is evaluation of the enthalpy and internal energy of a region or source, as described below. The overall scheme into which such an evaluation fits is:

1. Initialize State. Given initial conditions, initialize state variables: m_i and U .
2. Auxiliary Variables. Get temperature T , pressure P , and physical properties given state variables.
3. Rate Laws. Get rates-of-change for individual processes and assemble into overall derivatives of state variables.
4. Integration. Update state variables, and go to Step 2 above.

Initialization of state variables and calculation of auxiliary variables, the first two steps, are discussed under region thermodynamics below. These four steps are considered in greater detail when code architecture is discussed. Separate sections follow to discuss various transport phenomena contributing to rate laws: inter-compartmental flow, aerosol behavior, heat transfer to structures, and particle entrainment and de-entrainment.

2.2 Region Thermodynamics

Region thermodynamic models serve three functions:

1. Initialize state variables - mass and energy,
2. Compute pressure and temperatures, and
3. Compute aerosol formation/disappearance potential.

For temperatures and pressures of interest, a non-ideal gas model considering the second virial coefficient, temperature-dependent specific heats, and the non-ideal gas contribution to energy is excellent for treating water vapor, the least ideal of the gases. Thus, pressure is given by

$$\begin{aligned}
 P &= \sum P_i = \sum (R_i T) \left(\frac{1}{v_i} + \frac{B_i}{v_i^2} \right) \\
 &= (RT) \sum \left(\frac{n_i}{V} \right) \left(1 + \frac{B_i M_i n_i}{V} \right)
 \end{aligned}
 \tag{2-3}$$

where P = Initial pressure,
 T = Temperature,
 v = Specific volume,
 n = Mole fraction, and
 B = Second virial coefficient.

Given the initial pressure, temperature, and mole fractions, equation (2-3) is solved for the total gas moles and then the initial mass of each gas (m_i) follows. The initial energy is found by

$$U = \sum m_i u_i (T, v_i) = \sum m_i \{u_{i0} (T) + \Delta u_i (T, v_i)\} \quad (2-4)$$

where the term u_{i0} represents the integral of the temperature-dependent specific heat, including a reference value, and Δu_i represents the contribution arising from a nonzero B_i .

When mass and total energy are known, equation (2-4) is solved iteratively for the temperature, and subsequently equation (2-3) is solved for the pressure.

When aerosols are present, the term

$$\sum m_{ai} u_{ai} (T) \quad (2-5)$$

is added to the total energy. In general, the resulting temperature can represent a non-equilibrium state for vapor species, i.e., it may be true that the vapor pressure exceeds saturation, in which case aerosols (fog) should form, or it may be that aerosols exist but the calculated vapor pressure is less than saturation, in which case the aerosols should evaporate. Rates of aerosol formation and disappearance are discussed later, but the model requires the equilibrium state. The equilibrium state is found by solving equation (2-4) together with the constraints:

$$P_i \leq P_{sat,i} (T) \quad (2-6a)$$

$$m_{i,tot} = m_i + m_{ai} \quad (2-6b)$$

which means that the aerosol and gas masses are adjusted during the iteration for temperature, and the resulting equilibrium values are saved for reference by the aerosol models.

2.3 Heat Transfer

2.3.1 Finite Difference Solution for Heat Sink Temperature

HANSF includes models for heat transfer from a gas region to passive structural heat sinks such as the MCO walls or transfer casks, and conduction within the structure. Using an implicit finite difference formulation, the model solves the one-dimensional conduction equation subject to the boundary conditions specified for each heat sink surface. Pertinent features of the model are as follows:

- Heat sinks can be planar or cylindrical.
- Each heat sink can be subdivided into as many as 20 nodes.
- Heat sinks can be modeled as only one node (lumped capacitance).
- Volumetric heat generation can be included.

For a plane wall heat sink with constant thermal properties, the one-dimensional conduction equation is written as:

$$\frac{\partial^2 T}{\partial x^2} + \frac{Q}{k} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \quad (2-7)$$

where Q is the volumetric heat generation rate, k is the thermal conductivity, and α is the thermal diffusivity. For a cylinder with constant thermal properties, the one-dimensional conduction equation is:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{Q}{k} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \quad (2-8)$$

A finite difference formulation of either equation is:

$$A_n T_{n-1} + B_n T_n + C_n T_{n+1} = D_n \quad (2-9)$$

where, for an implicit solution, the temperatures are at the end of the time step. Expressions for coefficients, A, B, C, and D consider the following:

- Planar and cylindrical heat sinks,
- Non-uniform nodalization,
- Heterogeneous materials,
- Full or boundary half-nodes,
- Volumetric heat sources,
- External heat source to the boundary nodes,
- Convection, adiabatic, and fixed-temperature boundary conditions, and
- Gap resistance between two layers of a composite heat sink.

2.3.1.1 Discretization For Interior Nodes

Consider an interior node designated by index "i" and shown in Figure 2-1. Effective thermal resistance R_i between the centers of nodes "i" and "i + 1" is defined by,

$$Q_i = \frac{(T_i - T_{i+1})}{R_i} \quad (2-10)$$

where Q_i is net heat transfer rate from "i". For planar geometry, $A_i = A_{i-1} = A_{i+1}$ and clearly the effective resistance is given by:

$$R_i = \frac{\Delta x_i}{2A_i k_i} + \frac{\Delta x_{i+1}}{2A_i k_{i+1}} \quad (2-11a)$$

Likewise,

$$R_{i-1} = \frac{\Delta x_{i-1}}{2A_i k_{i-1}} + \frac{\Delta x_i}{2A_i k_i} \quad (2-11b)$$

Figure 2-1: Interior Heat Sink Node Discretization.

For cylindrical geometry, the heat conduction area varies linearly with distance and so does the resistance:

$$R_i = \int_{-\Delta x_i/2}^0 \frac{dx}{k_i \left(A_i + \frac{A_i - A_{i-1}}{\Delta x_i} x \right)} + \int_0^{\Delta x_{i+1}/2} \frac{dx}{k_{i+1} \left(A_i + \frac{A_i - A_{i-1}}{\Delta x_i} x \right)} \quad (2-12a)$$

or,

$$R_i = \frac{\Delta x_i}{A_i - A_{i-1}} \left[\frac{1}{k_{i+1}} \ln \left(1 + 0.5 \frac{\Delta x_{i+1}}{\Delta x_i} \left(1 - \frac{A_{i-1}}{A_i} \right) \right) - \frac{1}{k_i} \ln \left(1 - 0.5 \left(1 - \frac{A_{i-1}}{A_i} \right) \right) \right] \quad (2-12b)$$

Similarly,

$$R_{i-1} = \int_{-\Delta x_{i-1}/2}^0 \frac{dx}{k_{i-1} \left(A_{i-1} + \frac{A_i - A_{i-1}}{\Delta x_i} x \right)} + \int_0^{\Delta x_i/2} \frac{dx}{k_i \left(A_{i-1} + \frac{A_i - A_{i-1}}{\Delta x_i} x \right)} \quad (2-13a)$$

or,

$$R_{i-1} = \frac{\Delta x_i}{A_i - A_{i-1}} \left[\frac{1}{k_i} \ln \left(1 + 0.5 \left(\frac{A_i}{A_{i-1}} - 1 \right) \right) - \frac{1}{k_{i-1}} \ln \left(1 - 0.5 \frac{\Delta x_{i-1}}{\Delta x_i} \left(\frac{A_i}{A_{i-1}} - 1 \right) \right) \right] \quad (2-13b)$$

The energy balance around the node "i" is:

$$\rho_i V_i c_i \frac{(T_i - T_i^{\text{old}})}{\Delta t} = V_i Q''' + \frac{(T_{i-1} - T_i)}{R_{i-1}} - \frac{(T_i - T_{i+1})}{R_i} \quad (2-14)$$

After rearranging, the finite difference equation is obtained:

$$A_i T_{i-1} + B_i T_i + C_i T_{i+1} = D_i \quad (2-15)$$

$$\text{where } A_i = -1,$$

$$C_i = -R_{i-1} / R_i,$$

$$B_i = -A_i - C_i + R_{i-1} \rho_i V_i c_i / \Delta t, \text{ and}$$

$$D_i = R_{i-1} (\rho_i V_i c_i / \Delta t) T_i^{\text{old}} + R_{i-1} V_i Q'''$$

The volume V_i and the heat transfer area A_i need to be expressed in terms of the user inputs $XRI(IHS)$, $XRO(IHS)$, $AHS(IHS)$, and the node index "i". For heat sink IHS, XRI is the inner radius, XRO is the outer radius, and AHS is the surface area; for planar heat sinks, $XRI = 0.0$ and XRO is the thickness. As shown in Figure 2-2, normally a heat sink is nodalized with uniform node sizes, except for the boundary nodes which are half nodes.

Clearly, for planar geometry,

$$V_i = AHS(IHS) \Delta x_i \quad \text{for interior nodes,}$$

$$V_i = AHS(IHS) \Delta x_i / 2 \quad \text{for boundary nodes, and}$$

$$A_i = AHS(IHS).$$

For a cylindrical geometry, it is useful to define the equivalent height of the cylinder "L" such that

$$2\pi \frac{XRI(IHS) + XRO(IHS)}{2} L = AHS(IHS) \quad (2-16a)$$

or,

$$L = \frac{AHS(IHS)}{\pi (XRI(IHS) + XRO(IHS))} \quad (2-16b)$$

Now, the volume and heat transfer area of each node can be expressed as,

$$V_i = 2\pi r_i \Delta x_i L \quad \text{for interior nodes,} \quad (2-17a)$$

$$V_1 = \pi (XRO(IHS) - (\Delta x_1 / 4)) (\Delta x_1 / 2) L \quad \text{for an outer boundary node,} \quad (2-17b)$$

$$V_n = \pi (XRI(IHS) + (\Delta x_n / 4)) (\Delta x_n / 2) L \quad \text{for an inner boundary node,} \quad (2-17c)$$

$$\text{and } A_i = 2\pi (r_i - (\Delta x_i / 2)) L \quad (2-17d)$$

2.3.1.2 Discretization For Boundary Nodes

For boundary nodes, a heat conduction path is replaced by an appropriate boundary condition. Hence, the discretized equation for the outer boundary node is given by:

Figure 2-2: Boundary Half-Nodes.

$$\rho_1 V_1 c_1 \frac{(T_1 - T_1^{\text{old}})}{\Delta t} = V_1 Q''' - \frac{(T_1 - T_2)}{R_1} + S_{\text{outer}} + \frac{(T_{\infty, \text{outer}} - T_1)}{R_{\infty, \text{outer}}} \quad (2-18)$$

where S_{outer} is the external heat source to the outer surface of the heat sink and $R_{\infty, \text{outer}}$ and $T_{\infty, \text{outer}}$ characterize the convection boundary condition. The resistance is related to the convective heat transfer coefficient $h_{c, \text{outer}}$ by:

$$R_{\infty, \text{outer}} = \frac{1}{\text{ASHS (IHS, 2)} L h_{c, \text{outer}}} \quad (2-19)$$

where ASHS (IHS, 2) is the outer surface area. The adiabatic boundary condition can be specified by setting $R_{\infty, \text{outer}} = \infty$, and the fixed temperature boundary condition can be specified by setting $R_{\infty, \text{outer}} = 0$. Thus, for the outer boundary node, the coefficients of the discretized equation are reduced to:

$$\begin{aligned} A_1 &= 0, \\ C_1 &= -1, \\ B_1 &= -A_1 - C_1 + (R_1 / R_{\infty, \text{outer}}) + R_1 (\rho_1 V_1 c_1 / \Delta t), \text{ and} \\ D_1 &= R_1 (\rho_1 V_1 c_1 / \Delta t) T_1^{\text{old}} + R_1 (V_1 Q''' + S_{\text{outer}}) + (R_1 / R_{\infty, \text{outer}}) T_{\infty, \text{outer}} \end{aligned}$$

Similarly, the coefficients of the discretized equation for the inner boundary node are reduced to:

$$\begin{aligned} A_n &= -1, \\ C_n &= 0, \\ B_n &= -A_n - C_n + (R_{n-1} / R_{\infty, \text{outer}}) + R_{n-1} (\rho_n V_n c_n / \Delta t), \text{ and} \\ D_n &= R_{n-1} (\rho_n V_n c_n / \Delta t) T_n^{\text{old}} + R_{n-1} (V_n Q''' + S_{\text{inner}}) + \{R_{n-1} / R_{\infty, \text{inner}}\} T_{\infty, \text{inner}} \end{aligned}$$

2.3.1.3 Discretization For Composite Heat Sinks

Note that the last term in equation (2-18) resembles the usual conduction term on the inner side. In fact, if two heat sinks are joined together with a gap resistance between the two,

the discretized equations of the two heat sinks can be solved together as one contiguous heat sink by simply setting the $R_{\infty, \text{outer}}$ to the gap resistance, R_{gap} (see Figure 2-3). For this case, the coefficients of two heat sinks are joined together and the tridiagonal matrix solver is applied to the combined set of coefficients. The coefficients for the boundary nodes where the outer surface of heat sink A contacts the inner surface of heat sink B are as follows:

$$\begin{aligned} \text{For heat sink B,} \quad A_n &= -1, \\ C_n &= -R_{n-1} / R_{\text{gap}}, \\ B_n &= -A_n - C_n + R_{n-1} (\rho_n V_n c_n / \Delta t), \text{ and} \\ D_n &= R_{n-1} (\rho_n V_n c_n / \Delta t) T_n^{\text{old}} + R_{n-1} V_n Q''' \end{aligned}$$

$$\begin{aligned} \text{For heat sink A,} \quad A_1 &= -(R_1 / R_{\text{gap}}), \\ C_1 &= -1, \\ B_1 &= -A_1 - C_1 + R_1 (\rho_1 V_1 c_1 / \Delta t), \text{ and} \\ D_1 &= R_1 (\rho_1 V_1 c_1 / \Delta t) T_1^{\text{old}} + R_1 V_1 Q''' \end{aligned}$$

2.3.2 Heat Transfer to Heat Sink Surfaces

The finite difference scheme described above requires net heat transfer to inner and outer heat sink surfaces as part of the boundary conditions. First, it must be decided whether condensation can occur for any of the species in the region. For each gas, condensation occurs if:

$$P_{\text{sat}}(T_w) < \text{Min}(P_i, P_{\text{sat}}(T_g)) \quad (2-20)$$

where $P_{\text{sat}}(T_g)$ is the saturation pressure at the bulk gas temperature, $P_{\text{sat}}(T_w)$ is the saturation pressure at the wall temperature, and P_i is the partial pressure. A condensate layer is not explicitly tracked, and condensate is added to the region liquid, so that evaporation from a surface is not modeled here (special models for evaporation are employed for specific applications).

Figure 2-3: Composite Heat Sink.

If condensation cannot occur, heat transfer from the gas to the wall is based only on natural convection and radiation. A single heat transfer correlation is used:

$$Nu = 0.12 (Pr \cdot Gr)^{0.33} \quad (2-21)$$

where Pr is the Prandtl number, and Gr is the Grashof number. The Prandtl number is defined as,

$$Pr = \frac{\mu_g c_{pg}}{k_g} \quad (2-22)$$

where μ_g is the dynamic viscosity of the gas, c_{pg} is the specific heat of the gas, and k_g is the thermal conductivity of the gas. The Grashof number is

$$Gr = \frac{g \beta (T_w - T_g) L^3}{\left(\frac{\mu_g}{\rho_g} \right)^2} \quad (2-23)$$

where g is the acceleration of gravity, β is the ideal gas expansion coefficient, T_g is the gas temperature, T_w is the wall temperature, L is the heat sink characteristic dimension, and ρ_g is the gas density. The natural convection heat transfer coefficient is then:

$$h_c = \frac{Nu k_g}{L} \quad (2-24)$$

Radiation heat transfer from the gas to the heat sink is described by the following heat transfer coefficient:

$$h_r = \sigma \epsilon (T_g^2 + T_w^2) (T_g + T_w) \quad (2-25)$$

where σ is the Stefan-Boltzmann constant, and ϵ is the heat sink emissivity. Net heat transfer to the heat sink is then:

$$Q_w = (h_c + h_r) A (T_g - T_w) \quad (2-26)$$

where A is the heat sink one-sided surface area.

If condensation occurs, the condensate film interface temperature is found iteratively. The gas-to-interface heat transfer rate must be equal to the sum of the conduction heat transfer rate through the liquid and the energy carried by the film:

$$Q_g (T_f) = Q_w (T_f) + Q_f (T_f) \quad (2-27)$$

where Q_g is the heat transfer from the gas to the film, including convection, radiation, and condensation; Q_w is conduction through the liquid layer; and Q_f is the energy carried away by the film. The evaporation rate is given by the Chilton-Colburn analogy:

$$h_m = \frac{h_c}{c_{pg}} \left(\frac{D}{\alpha} \right)^{\frac{2}{3}} \quad (2-28a)$$

$$\dot{m}'' = h_m \ln (1 + B) = h_m (Y_s - Y_\infty) \quad (2-28b)$$

$$B = \frac{Y_s - Y_\infty}{1 - Y_s} \quad (2-28c)$$

where D = Binary diffusion coefficient, m^2/s ,

α = Thermal diffusivity, m^2/s ,

h_m = Mass transfer coefficient, $kg/m^2 \cdot s$,

$\dot{m}''$ = Condensation flux, $kg/m^2 \cdot s$,

Y_s = Mass fraction of vapor evaluated at surface (water film) temperature, and

Y_∞ = Bulk vapor mass fraction.

2.4 Aerosol Model

Aerosol transport and deposition are modeled via mass balance equations for the total aerosol mass in each control volume. The particle size distribution of aerosols is considered implicitly by the deposition models through a correlation technique [Epstein and Ellison, 1988]

as explained below. Validation of the method is abundantly described in the references [Vaughan and von Arx, 1988].

The mass balance of aerosols of compound i is written

$$\frac{dm_i}{dt} = -\lambda_{\text{dep}} m_i - \lambda_{\text{out}} m_i + \sum \lambda_{\text{in}} m_{i,\text{don}} + S_i \quad (2-29)$$

where m_i = Mass of aerosol compound i , kg,
 λ_{dep} = Deposition rate constant, 1/s,
 λ_{out} = Outflow rate constant, 1/s,
 λ_{in} = Inflow rate constant on a given flow path, 1/s,
 $m_{i,\text{don}}$ = Donor region aerosol mass, kg, and
 S_i = Source, kg/s.

Note that, when required, information on the particle size is encoded into λ_{dep} .

For transport between volumes, the rate constant is simply the fractional volumetric flow rate, hence, it is independent of particle size:

$$\lambda_{\text{out}} = \frac{W_g}{\rho_g V_{\text{don}}} \quad (2-30)$$

where W_g = Flow rate along path, kg/s,
 ρ_g = Density, kg/m³, and
 V_{don} = Volume of donor region, m³.

The equation applies for inflow and outflow.

Aerosol deposition in tanks occurs by condensation and sedimentation. Condensation removal is independent of particle size and is written as

$$\lambda_{\text{cond}} = \frac{W_{\text{cond}}}{\rho_g V} \quad (2-31)$$

Aerosol sedimentation is particle-size dependent and correlations that implicitly account for particle size are used for two dimensionless rate constants, chosen based on the source strength [Epstein and Ellison, 1988]:

$$\lambda_{sed}^{ss} = C_{\lambda} \Lambda_{sed}^{ss} \quad (2-32a)$$

$$\lambda_{sed}^D = C_{\lambda} \Lambda_{sed}^D \quad (2-32b)$$

where λ_{sed}^{ss} = Steady-state sedimentation rate,
 λ_{sed}^D = Decay sedimentation rate,
 C_{λ} = Scaling factor for λ , and
 Λ = Dimensionless sedimentation rate.

2.5 Gas Flow Model

Gas flow between compartments or to the environment is calculated using the standard compressible flow equation for pressure-driven flow and accounting for the possibility of choking. A rather complex numerical scheme is employed to assure numerical stability because multiple flow paths may exist from a given region (for example, there may be several vent lines on a tank). Flow occurs between the region of higher upstream pressure P_{up} to the region of lower downstream pressure P_{dn} and is choked when the pressure ratio P_{up}/P_{dn} is less than the critical pressure ratio:

$$r_{crit} = \left(\frac{2}{1 + \gamma} \right)^{\frac{\gamma}{\gamma - 1}} \quad (2-33)$$

The pressure ratio used is the minimum:

$$r = \min (r_{crit}, P_{dn}/P_{up}) \quad (2-34)$$

and the mass flowrate is given by:

$$W_j = C_o A \left[\frac{2\gamma P_{up} \rho}{\gamma - 1} r^{2/\gamma} \left(1 - r^{\frac{\gamma-1}{\gamma}} \right) \right]^{\frac{1}{2}} \quad (2-35)$$

where C_o is the loss coefficient and γ and ρ are upstream quantities.

All flowrates through junctions between regions are solved simultaneously by recasting the single-junction flow equation as

$$P_{upj} - P_{dnj} = K_j W_j |W_j| \quad (2-36)$$

where the effective coefficient K_j is derived from the compressible formula for W_j and the known pressure difference. Flowrates are found so that the equation above is true for end of timestep pressures, for example,

$$P_{upj} = P \left(m_{upj}^{ex}, U_{upj}^{ex} \right) - \rho_{upj}^{ex} g z_{upj} \quad (2-37)$$

where the superscript ex indicates an extrapolated value and the pressure in the region is corrected for static head at the junction elevation through the second term.

Extrapolated gas masses and energies are found by incrementing the beginning of timestep values using known source rates and the current guess for the flowrate of each junction. Extrapolated pressure and temperature are found by the same technique normally used for a control volume. Newton's method is used to converge on the flowrates.

2.6 Counter-Current Flow

Counter-current volumetric flowrate Q_{cc} generally depends on the density difference, the flow orientation (vertical or horizontal), and the length-to-diameter ratio L/D of the flowpath. The net exchange of a gas W_{cci} is given by:

$$W_{cci} = Q_{cc} (c_{i1} - c_{i2}) \quad (2-38)$$

where c_{i1} and c_{i2} are concentrations of gas (or aerosol) in the two compartments exchanging gases. Clearly, counter-current flow must be considered whenever a gas or aerosol is abundant in one region, but depleted in another region connected by a junction.

HANSF calculates the buoyancy-driven, counter-current exchange flow, Q_{cc} , and the purging flow rate, q , across a junction and outputs the mass flow rates corresponding to these volumetric flow rates. These can be determined for any of four junction types: 1) a rectangular horizontal junction, 2) a rectangular vertical junction, 3) a circular horizontal junction, and 4) a circular vertical junction.

2.6.1 Horizontal Walls

Calculation of pure counter current flow through a rectangular junction in a horizontal wall is based on [Epstein, 1988]:

$$\frac{Q_{cc}}{(D^5 g \Delta \rho / \bar{\rho})^{1/2}} = \frac{0.055[1 + 400 (L/D)^3]^{1/6}}{\{1 + 0.00527[1 + 400 (L/D)^3]^{1/2} [(L/D)^6 + 117 (L/D)^2]^{3/4}\}^{1/3}} \quad (2-39)$$

where D = Junction diameter,
 g = Acceleration of gravity,
 $\Delta \rho$ = Density difference,
 $\bar{\rho}$ = Average density, and
 L/D = Length-to-diameter ratio.

The flooding flow rate through this junction is:

$$\frac{q}{(D^5 g \Delta \rho / \bar{\rho})^{1/2}} = \frac{0.19[1 + 4 \cdot 10^3 (L/D)^3]^{1/9}}{\{1 + 5.091 \cdot 10^{-2} (L/D)^{16/7} [1 + 4 \cdot 10^3 (L/D)^3]^{4/9}\}^{1/4}} \quad (2-40)$$

These equations are applied to both rectangular and circular openings in horizontal walls. This is possible since the volume exchange rate, in these equations, is appropriately expressed in terms of the Froude number $Q/(D^5 g \Delta \rho / \bar{\rho})^{1/2}$, and the Froude number is only a function of the

length-to-diameter ratio of the opening. The parameter range for which these equations are known to be valid base on experimental evidence is:

$$0.01 < L/D < 20 \quad \text{and} \quad 0.025 < \Delta\rho/\bar{\rho} < 0.17 \quad (2-41)$$

but the correlation should be valid to higher values of $\Delta\rho/\bar{\rho}$.

2.6.2 Vertical Walls

Pure counter-current flow through a rectangular junction in a vertical wall is based on:

$$\frac{Q_{\infty}}{\sqrt{W^2 H^3 g \Delta\rho/\bar{\rho}}} = \frac{C_D}{3} \quad (2-42)$$

where W is junction width and H is junction height.

The flooding flow rate through this junction is:

$$q = 2^{3/2} Q_{\infty} = \frac{2 C_D}{3} \sqrt{\frac{2 W^2 H^3 g \Delta\rho}{\bar{\rho}}} \quad (2-43)$$

Pure counter-current flow through a circular junction in a vertical wall is:

$$\frac{Q_{\infty}}{\sqrt{D^5 g \Delta\rho/\bar{\rho}}} = 0.24 C_D \quad (2-44)$$

The flooding flow rate through this junction is:

$$q = 3.143 Q_{\infty} = 0.75 C_D \sqrt{D^5 g \Delta\rho/\bar{\rho}} \quad (2-45)$$

2.6.3 Combined Forced and Natural Convection Flow in Horizontal Walls

The combined effect of natural convection and forced flow through an opening in a horizontal wall has the power-law form:

$$Q_{BF} = Q_{cc} (1 - Q_u/q)^{2.3} \quad (2-46)$$

where Q_u is pressure-driven uni-directional flow. The buoyancy-driven component of the combined convection across a horizontal junction is calculated to an accuracy of 25% by this expression.

2.6.4 Combined Forced and Natural Convection Flow in Vertical Walls

The combined effect of natural convection and forced flow through openings in a vertical wall have power-law forms which are similar to the empirically determined expressions for flow through horizontal partitions:

$$Q_{BF} = Q_{cc} (1 - Q_u/q)^{3/2} \quad (2-47)$$

Combined flow through a circular opening in a vertical wall is:

$$Q_{BF} = Q_{cc} (1 - Q_u/q)^{1.6} \quad (2-48)$$

2.7 Entrainment

Sludge particles can be released from the MCO by entrainment of particles deposited on the fuel assemblies and scrap basket. Resuspension is expressed by the rate parameter, Λ , which is defined as follows:

$$\Lambda = \frac{M}{\chi A t} \quad (2-49)$$

where M is the resuspended mass (kg), χ is the surface mass concentration (kg/m²), A is the surface area (m²), and t is time in seconds.

Reynolds and Slinn recommend the following empirical correlation for resuspension from a dry, gravel substrate [Reynolds and Slinn, 1979]:

$$\Lambda = 7.39 \cdot 10^{-10} U^3 \quad (2-50)$$

where U is the gas velocity in m/s. Measurements made by Sehmel suggest that for smooth aluminum surfaces, however, the resuspension parameter is three orders of magnitude higher than the resuspension parameter for dry gravel [Sehmel, 1975]. Therefore, the constant in equation (2-50) is multiplied by the geometric mean of 10^3 and 10^4 ($10^{3.5}$) to obtain the following:

$$\Lambda = 2 \cdot 10^{-6} U^3 \quad (2-51)$$

For conservatism, this expression is used in HANSF; it overstates resuspension by assuming that all surfaces in the MCO are smooth.

The HANSF code calculates the appropriate gas velocity by taking into account the mass flowrate leaving the region (MCO), the gas density, and the flow area available through the fuel assembly or scrap basket. Resuspended mass is added to the UO₂ aerosol mass in the region, and decremented from the sludge mass on the fuel assembly and scrap basket surfaces. At present, resuspension is not considered in junctions or surfaces other than the fuel assemblies or scrap basket.

2.8 De-Entrainment

Airborne particles can be de-entrained from a gas flow and deposited in the scrap basket, or at bends and elbows in junctions. For 90 degree bends, the experimental results of Pui [Pui, et al., 1987] are used to calculate the amount deposited. Pui expresses the deposition efficiency (mass fraction deposited) for one 90 degree bend as follows:

$$n = 1 - 10^{-0.963 St} \quad (2-52)$$

where St is the Stokes number. The Stokes number is:

$$St = \frac{C \rho_p D_p^2 U}{18 \mu a} \quad (2-53)$$

where C is the slip correction factor, ρ_p is particle density, D_p is the particle diameter, U is the gas velocity in the junction, μ is the absolute viscosity of the fluid, and a is the radius of the junction. Because the Stokes number is a function of particle size, Pui's expression must be evaluated over a range of particle sizes. HANSF uses 30 bins to describe the aerosol size distribution; Pui's expression is evaluated for each bin to determine the total aerosol mass deposited.

The scrap basket provides a significant flowpath through the MCO, but inertial impaction removes entrained particles from the gas stream. Particles in the gas stream would be impacted against the scrap basket rubble because of their inertia. Jackson and Calvert [Jackson and Calvert, 1966] developed a simple relation for particle collection in packed beds, based on the inertial impaction parameter K :

$$K = \frac{\rho_p U_s D_p}{9 \mu B} \quad (2-54)$$

where ρ_p is the particle density, U_s is the gas velocity in the scrap basket, D_p is the particle diameter, and B is the width of the flow channel. For packed beds, Jackson and Calvert

estimated that $B = 0.1 D$, where D is the diameter of the packing. For turbulent or laminar flow, the collection efficiency is

$$E = 1 - \exp(-\pi n K) \quad (2-55)$$

where n is the number of 360 degree turns made by the gas. This is simply:

$$n = \frac{Z}{2D} \quad (2-56)$$

where Z is the height of the packed bed, or scrap basket in this case. Because K depends on particle size, equation (2-54) is evaluated for each of the 30 particle size bins used by HANSF.

2.9 Properties

Gas and liquid mixture thermal properties must be appropriate weighted-averages of the thermal properties of the individual species. Consider mixture values for gases first. Gas mixture specific heat is simply a mass-averaged value of all constituents. Mixture thermal conductivity is from [Bird, et al., 1960]:

$$K_{\text{mix}} = \frac{\sum_{i=1}^n x_i K_i}{\sum_{j=1}^n x_j \Phi_{ij}} \quad (2-57)$$

where x is mole fraction and k is the thermal conductivity of the individual species. Coefficients Φ_{ij} are defined by:

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-\frac{1}{2}} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \left(\frac{M_j}{M_i} \right)^{\frac{1}{4}} \right]^2 \quad (2-58)$$

where M is molecular weight and μ is dynamic viscosity at system pressure and temperature.

Brokaw's approximation gives gas-mixture dynamic viscosity, μ_{mix} :

$$\mu_{\text{mix}} = \frac{\sum_{i=1}^n x_i \mu_i}{\sum_{j=1}^n \mu_j \Phi_{ij}} \quad (2-59)$$

where $\Phi_{ij} = \sqrt{\frac{\mu_i}{\mu_j}} S_{ij} A_{ij}$, and (2-60)

$$A_{ij} = \left(\frac{M_i}{M_j} \right)^{-0.37} \quad (2-61)$$

For non-polar gases, $S_{ij} = 1.0$. For polar gases,

$$S_{ij} = \frac{1 + (T_i^* T_j^*)^{\frac{1}{2}} + \left(\frac{\delta_i \delta_j}{4} \right)}{\left[1 + T_i^* + \frac{\delta_i^2}{4} \right]^{\frac{1}{2}} \left[1 + T_j^* + \frac{\delta_j^2}{4} \right]^{\frac{1}{2}}} \quad (2-62)$$

and

$$T^* = \frac{k T}{\epsilon} \quad (2-63)$$

where k is Boltzmann's constant and ϵ is the characteristic energy. δ is a polar parameter

$$\delta = \frac{\mu_p^2}{2 \epsilon \sigma^3} \quad (2-64)$$

where μ_p is the dipole moment and σ is a parameter for an intermolecular potential function, such as the Lennard-Jones 12-6 potential. Values of ϵ/k , δ , and σ (Stockmayer-Potential Parameters) are tabulated for various gases [Reid, et al., 1977], and must be included as part of the input for each species.

Liquid (condensate film) properties must be appropriate averages based on the pure liquid properties. Condensate film mixture specific heat, latent heat of vaporization, and specific

volume are based on a mass fraction weighted-average. For example, the specific heat of the film mixture is:

$$C_{pe} = \sum_{j=1}^N C_{pej} x_j \quad (2-65)$$

$$\text{where } x_j = \frac{W_{ej}}{\sum_{j=1}^N W_{ej}} \quad (2-66)$$

Film mixture values for kinematic viscosity and thermal conductivity are slightly more complicated. Film mixture kinematic viscosity is based on a mole fraction weighted-average:

$$\nu_e = \exp \left\{ \sum_{j=1}^N n_j \log \nu_{ej} \right\} \quad (2-67)$$

where n_j is defined as,

$$n_j = \frac{\frac{W_{ej}}{M_j}}{\sum_{j=1}^N \frac{W_{ej}}{M_j}} \quad (2-68)$$

The Li equation gives the film mixture thermal conductivity [Reid, et al., 1977]:

$$k_e = \sum_{i=1}^N \sum_{j=1}^N \phi_i \phi_j k_{eij} \quad (2-69)$$

$$\text{where } k_{eij} = \frac{2}{\frac{1}{k_{ei}} + \frac{1}{k_{ej}}} \quad (2-70)$$

and ϕ_i (or ϕ_j) is the volume fraction of pure liquid i (or j). Volume fraction is given by:

$$\phi_i = \frac{n_i \frac{M_i}{\rho_{ei}}}{\sum_{i=1}^N \frac{n_i M_i}{\rho_{ei}}} \quad (2-71)$$

3.0 MCO MODELS

General MCO phenomena models are discussed here. Generic models, such as those for gas flow or aerosol behavior, are described in the previous section.

3.1 MCO Description

An MCO is a right circular cylinder comprised of stainless steel (Figure 3-1) with a welded flat bottom, circular head, and an elaborate top head known as the shield plug which contains all penetrations to the MCO interior (Figure 3-2) [Goldmann, 1997]. An MCO holds five tiers of baskets containing either re-racked fuel or scrap. Double annular fuel assemblies are re-racked into a honeycomb pattern with 54 assemblies per basket, as shown in Figures 3-3 and 3-4. Fuel too damaged for a fuel basket is placed in a scrap basket, Figure 3-5. Scrap baskets have six equally spaced radial spokes for integrity and these spokes, the outer wall, and a circular interior divider, are copper-lined for heat transfer. The interior division provides a location for so-called fine scrap pieces.

The MCO wall is a 24" (610 mm) diameter stainless steel pipe with a 0.500" (12.7 mm) wall thickness. The MCO has a 1.75" (45 mm) thick stainless steel bottom and a 3.5" (89 mm) thick stainless steel lid. About 3" below the lid is an 8.0" (203 mm) thick stainless steel shield plug. Two 1" valved piping connections terminate between the MCO lid and shield plug. These provide for venting from the top of the MCO and draining/filling via a filtered dip tube which extends almost to the MCO bottom. The overall MCO height is 13'-9.25" (4.197 m) while the inside (gas space) height from the MCO bottom to the shield plug is 11'-8.4" (3.566 m). Fuel and scrap basket center posts, or inserts, are centered on the filtered dip tube, also called the process guide tube, that runs from the shield plug to almost the MCO bottom. Fuel basket inserts have an outer diameter of 2.75" (69.9 mm), inner diameter of 1.75" (44.5 mm), and height of 27.317" (694 mm). Scrap basket inserts are slightly longer at 27.82" (707 mm), but

Figure 3-1A: MCO Top Portion With Shield Plug and Cover.

Figure 3-1B: MCO Bottom Portion.

Figure 3-2: MCO Shield Plug.

Figure 3-3: Mark IV Fuel Basket.

Figure 3-4: Base Plate Assembly and Dimensions.

Figure 3-5A: Scrap Basket Configuration.

Figure 3-5B: Scrap Basket Configuration.

PARTS/MATERIAL LIST						
QTY REQD	PART/DASH NUMBER	DESCRIPTION	MATERIAL/REFERENCE	SHEET	REV	NO
1	-010	ASSEMBLY		1	1	1
1	-020	SUBASSEMBLY, BASEPLATE & CENTER POST		3	2	2
1	-030	SUBASSEMBLY, COPPER SHIELD SECTIONS		2	3	3
					4	4
					5	5
6	-001	SUPPORT ROD, BAR #1.313"	ASTM A-479 304L SST	1	6	6
1	-002	BOTTOM SCREEN	304 SST	3	7	7
1	-003	CENTER POST, #2.75" OD x .50" WALL	ASTM A-312 TP 304L SST	2	8	8
1	-004	BUSHING, #4.00" OD x 0.8425" WALL	ASTM A-479 304L SST	2	9	9
1	-005	BASE PLATE, #22.825" x 1.23" THK	ASTM A-240 304L SST	2	10	10
6	-006	SHIELD, 60° SEGMENT, 29.32" x 26.25" x .125" THK	ASTM B-152 UNS C12200-060	3	11	11
1	-009	FLOW RESTRICTOR, .013 THK x 6 x .71	ASTM B-103 UNS C51000-H08	3	12	12
					13	13
					14	14
6		.500 COILED TYPE SPRING PIN x 2.0" LONG	SAE 30302 OR 30304 AMS/ASME B18.8.2-94	1	15	15
6		BACKING ROD, COPPER, 5/32 DIA.	ERCU, AMS A5.7-84R	3	16	16
12		FLUSH HEAD BLIND RIVET, SERIES M0.4, RIVET NO. 43	GRADE 51, 91-114	3	17	17

GENERAL NOTES: (UNLESS OTHERWISE SPECIFIED)

- ALL PARTS AND MATERIAL AS SPECIFIED OR ENGINEERING APPROVED EQUAL.
- ABBREVIATIONS ARE IN ACCORDANCE WITH AMS/ASME Y1.1-88.
- WELDING SYMBOLS ARE IN ACCORDANCE WITH AMS/AWS A2.4-83.
- SURFACE TEXTURE SYMBOLS ARE IN ACCORDANCE WITH AMS/ASME Y14.38-86. SURFACE TEXTURE VALUES ARE IN MICROINCHES AND ARE IN ACCORDANCE WITH AMS/ASME B46.1-85.
- ALL UNSPECIFIED MACHINED SURFACES SHALL BE $\sqrt{}$ OR BETTER IN ACCORDANCE WITH AMS B46.1.
- REMOVE ALL BURRS AND BREAK ALL SHARP EDGES.
- ALL UNSPECIFIED MACHINE TOOL RADI SHALL BE .03 MAXIMUM.
- WELDED SURFACES SHALL BE SMOOTH AND UNIFORM IN APPEARANCE WITHOUT ABRUPT CHANGES IN CONTOUR.
- DIMENSIONING AND TOLERANCING SHALL BE PER AMS/ASME Y14.5M-82. DIMENSIONS ARE IN INCHES AND APPLY AT 72° UNLESS OTHERWISE SPECIFIED. UNSPECIFIED TOLERANCES SHALL BE:
 -DECIMAL: .X ±.1, .XX ±.03, .XXX ±.005
 -ANGULAR: .1°
 -ALL IMPLIED 90° ANGLES SHALL BE PERPENDICULAR WITHIN THE GREATEST TOLERANCE OF THE LINEAR DIMENSION.
 -ALL COAXIAL FEATURES SHALL BE CONCENTRIC WITHIN .003 UNLESS OTHERWISE SPECIFIED.
- APPROXIMATE WEIGHT = 415 LB
- FABRICATION, WELDING AND INSPECTION SHALL BE IN ACCORDANCE WITH AMS-SE-888-1-88 DIVISION 1- SUBSECTION HQ AND SECTION 1- THE COPPER SHIELD ASSEMBLY IS A NON-BOGE ITEM AND IS EXEMPT FROM BOGE REQUIREMENTS.
- ADDITIONAL FABRICATION REQUIREMENTS ARE IN HWF-S-0453, FABRICATION SPECIFICATION FOR MULTI-CANISTER OVERPACK.
- PIECE/PART TOLERANCES ON THESE DRAWINGS SHOULD LEAD TO ACCEPTABLE ASSEMBLY GEOMETRIES. ALTERNATE PIECE/PART TOLERANCES MAY BE UTILIZED WITH THE BUYER'S APPROVAL. ACCEPTABLE FINAL ASSEMBLY GEOMETRIES ARE SHOWN IN THE FABRICATION SPECIFICATION'S CRITICAL DIMENSION TABLES/SKETCHES. IN THE EVENT THAT THERE IS A CONFLICT BETWEEN THE CRITICAL DIMENSION TABLES/SKETCHES AND THE DESIGN DRAWING, THE BUYER SHALL BE NOTIFIED FOR RESOLUTION.

otherwise the same. The process guide tube is 147.95" (3758 mm) long, with an outer diameter of 1.315" (33.4 mm) and inner diameter of 0.599" (15.2 mm).

The MCO is placed in a transfer cask during shipping and handling or a vault tube during long term storage. The carbon steel cask wall is 8" (203 mm) thick and the air gap between the MCO and cask (or vault tube) wall is about 1.0" (25 mm) thick. Key fuel and MCO/cask dimensions are summarized in Table 3-1.

Table 3-1: Key Fuel and MCO/Cask Dimensions	
Fuel Assembly	
Inner Diameter of Inner Ring, m	0.0122
Outer Diameter of Inner Ring, m	0.0325
Inner Diameter of Outer Ring, m	0.0432
Outer Diameter of Outer Ring, m	0.0616
Length of Inner Cylinder of a Fuel Assembly, m	0.661
Length of Outer Cylinder of a Fuel Assembly, m	0.663
Number of Fuel Assemblies in an MCO Tier	54
Number of Tiers in an MCO	5
MCO	
Inner Diameter, m	0.584
Wall Thickness, m	0.0127
Inside Height from MCO Bottom to Shield Plug, m	3.566
Transfer Cask	
Wall Thickness, m	0.203
Air Gap Thickness, m	0.025
Height, m	4.407
Dip Tube	
Outer Radius, m	0.0167
Inner Radius, m	0.0076
Insert	
Outer Radius, m	0.0349
Inner Radius, m	0.0175

3.2 Nodalization and Assumptions

Compartments (gas nodes) considered might include the MCO gas space(s), the air gap between the MCO and staging tube/cask walls, and the environment. An MCO interior may be modeled as consisting of anywhere from one to five tiers, where a tier is a fuel basket or scrap basket or represents more than one basket in a single "lumped" basket. In this manner, the user can model axial variations in the MCO interior, such as different reaction areas, decay heats, etc., between fuel baskets. Figure 3-6 is an example of four fuel baskets with one scrap basket. Up to two scrap baskets are allowed. The MCO free volume should be modeled using one gas node per basket to further capture axial variations in the MCO. For example, for Figure 3-6, the MCO interior can be modeled as five gas spaces; one for the scrap basket and one for each fuel basket. The user specifies the gas volume that each fuel basket or scrap basket is located in by specifying boundary conditions for each fuel element. These gas volumes would then communicate via flow areas set by the user through generic junction inputs. Forced flows into or out of MCO gas volumes can be imposed, so as to model recirculation of helium or nitrogen.

In the base model, fuel basket, MCO wall, and cask wall are nodalized radially as illustrated in Figure 3-7. Thermal analysis can efficiently take advantage of symmetry, such that the fuel may be represented by 14 heat sinks in a 30° sector of the MCO. Thus, seven pairs of heat sinks are used to represent the portions of seven fuel assemblies located in that sector. Each of these solid nodes constitutes a heat sink which may have an associated water mass on it. Water which is initially present on a fuel node typically evaporates as the node heats up and then condenses on cooler fuel or on the MCO wall. As cooler fuel or the MCO wall heats up, this condensed water subsequently re-evaporates. Water vapor and oxygen can participate in oxidation of fuel and, if the MCO is not sealed, these gases may be convected to (and from) the environment.

A scrap basket is modeled in a pseudo-one-dimensional manner illustrated in Figure 3-8. As shown in Section 3.7.2 below, the exact solution for the scrap temperature distribution may be well-represented by identifying the dominant heat flow paths as either azimuthal or radial.

Figure 3-6: MCO Control Volumes and Flowpaths.

Figure 3-7: Pin-by-Pin Nodalization Scheme.

Figure 3-8: Sample Scrap Basket Nodalization.

○ Example heat sink indexing scheme.

SL991041.CDR 1-25-99

These heat transfer paths are constructed by the user on input, as discussed in Section 5. As with fuel baskets, evaporation and oxidation are considered in the scrap, but because of the scrap debris bed geometry, a distributed solution is found for the temperature in each scrap heat sink, as described later. Fuel and scrap baskets are situated within the MCO by a center post (insert) placed around a process guide tube (long dip tube) that runs from the shield plug to the bottom shell. Because a 0.7 mm air gap separates the insert from the long dip tube, the two can be modeled as a composite heat sink with two layers and some gap resistance. The insert then provides a fin conduction path from the fuel and scrap baskets to the shield plug. Water mass on the insert is tracked, meaning that an initial water mass on the insert is specified and evaporation/condensation are considered.

Global natural circulation inside a sealed MCO is assumed to be negligible, based on an assessment of buoyancy driven flow in a porous medium with internal heat generation, i.e., Section 1.10. Local natural circulation, say in the tall vertical spaces between fuel assemblies, is accounted for, although heat removal from the MCO is generally dominated by radiation and conduction mechanisms. Note that although global natural circulation heat transfer is neglected, the MCO gas spaces are still assumed to be well-mixed such that oxygen and steam, if present, are readily available to all fuel nodes. In the absence of global convection, gas in an MCO would locally assume a mean temperature between the temperatures of the adjacent structures.

3.3 Oxidation of Fuel

In the presence of liquid water, oxygen, and/or steam, exposed uranium metal surfaces and the uranium hydride particles corrode by taking up the oxygen. Corrosion in an oxidizing atmosphere is modeled, but corrosion of submerged fuel is not considered at present.

When both oxygen and steam are present, the fuel reacts preferentially with oxygen. Once the oxygen is depleted, steam starts to react with the fuel. The heat produced by these exothermic reactions is deposited on the fuel, and the gaseous product, hydrogen, leaves the

surface at the fuel temperature. Reactions and their heats of reaction considered in the model are as follows:

When oxygen is present:

or

In an oxygen-free environment:

In the reactions above, U may be either original metal or dehydrided hydride. The uranium hydride-oxygen reaction to produce water vapor is favored by free energy over the reaction to produce hydrogen. The fraction of the oxygen reacting with uranium hydride which produces hydrogen instead of water vapor is a user-input model parameter FO2HYH2.

Reaction rates are usually expressed in terms of mass of oxygen uptake rate per unit area (i.e., mg/cm²-hr or kg/m²-s). A number of experimental investigations and derived reaction rate laws appear in the literature for unirradiated, uncorroded U metal reaction with O₂ and/or H₂O. The same rate law is assumed to apply for oxidation of uranium hydride. However, the reaction area of the hydride would normally be much higher than for pure uranium since UH₃ exists in particulate form, which explains why hydrides tend to be pyrophoric. Likewise, corroded fuel has larger reaction areas due to cracks and crevices. In order to account for these enhancing effects, the code calculates the oxidation rate in the following way:

1. The user chooses one of the literature rate law for unirradiated, uncorroded uranium.
2. For fuel elements, the user specifies the fraction of geometric surface that is exposed for oxidation (i.e., decladded area). Then, an oxidation multiplier is specified that accounts for surface irregularities, irradiation, uncertainties, etc. Therefore, the oxidation rate in a fuel node is given by:

$$F_{ox} = R_{ox} f_{multiplier} f_{exposed} A_{geometric} \quad (3-1)$$

where: F_{ox} = oxidation rate (kg of oxygen uptake per second),
 R_{ox} = rate law (kg/m²-s),
 $f_{multiplier}$ = oxidation multiplier,
 $f_{exposed}$ = fraction of geometric area exposed for oxidation (i.e., decladded), and
 $A_{geometric}$ = geometric area (m²).

3. For the scrap basket, the user specifies the geometric surface area available for oxidation per unit volume (bulk) of scrap. Then, a scrap basket oxidation multiplier is specified. Therefore, the oxidation rate in a scrap node is given by:

$$F_{ox} = R_{ox} f_{multiplier} A_v V_{scrap} \quad (3-2)$$

where: F_{ox} = oxidation rate (kg of oxygen uptake per second),
 R_{ox} = rate law (kg/m²-s),
 $f_{multiplier}$ = oxidation multiplier,
 A_v = exposed area per volume of the scrap (m⁻¹), and
 V_{scrap} = bulk volume of the scrap (m³).

4. For hydride particles, the user specifies their average diameter. Then, the initial inventory of uranium hydride in both the fuel basket and scrap basket is determined by specifying the initial oxide thickness on the exposed surface area and fraction of the oxide which is hydride. Note that the oxidation multiplier is not applied to the hydride particles. Therefore, the oxidation rate of hydride particles is given by:

$$F_{ox} = R_{ox} \frac{6}{d_{hyd}} f_{hyd} t_{ox} f_{exposed} A_{geometric} \quad \text{for hydrides in the fuel basket} \quad (3-3a)$$

$$F_{ox} = R_{ox} \frac{6}{d_{hyd}} f_{hyd} t_{ox} A_v V_{scrap} \quad \text{for hydrides in the scrap basket (3-3b)}$$

where: d_{hyd} = the diameter of the hydride particle,
 f_{hyd} = the fraction of hydride in the oxide, and
 t_{ox} = the initial oxide thickness.

The code tracks depletion of hydride particles as they oxidize. As the mass of hydride decreases, the reaction area is reduced, and the oxidation rate of hydride decreases accordingly. However, new hydride particles imbedded in the fuel matrix may be exposed as fuel oxidizes and layers peel off. The user has an option to fix the reaction area to the initial value by setting the model parameter IHYDKP to one. When IHYDKP = 2 option is invoked, a constant reaction area is used until all hydride is depleted, at which point the reaction area becomes zero.

One of three choices of oxidation rate laws is used by the code, depending on the user's choice. One choice is simply to use Trimble's correlation for all conditions [Trimble and Welsh, 1998]. Another choice of oxidation rate laws uses the McGillivray correlation for an oxygen and steam environment [McGillivray, et al., 1994], and the Ritchie correlation for a pure steam environment [Ritchie, 1981]. In the event that all oxygen is consumed or purged (say by vapor generation in a vented MCO), the Ritchie law is used. An alternative set of rate laws based on the Pearce correlation can be invoked by the user. Oxidation rate laws are summarized in Table 3-2 and Figure 3-9. The temperature used in the rate laws is bounded by 0°C and 1000°C. In Table 3-2, "Oxygen-Free" means that the mole fraction of O₂ is less than or equal to 1%, and "Dry" means that the partial pressure of steam is less than or equal to 1.5 Pa. The term "100% RH" means that the relative humidity of steam is greater than or equal to 0.999, as a practical matter. The user can specify whether both covered and uncovered fuel surface react with steam in the free steam (IOXDTN = 1) or the covered surface reacts with water (IOXDTN = 2). For reaction with water, P_{st} in the rate law represents the saturation pressure at the fuel surface temperature. Otherwise, P_{st} is the partial pressure of steam in the free stream.

Table 3-2: Oxidation Rate Law Summary

Conditions	Source	Correlation (3, 4)
(a) Oxygen-Free Steam	Ritchie (1)	$\frac{32.0}{238.0} 3.28E8 \exp \left(\frac{-13,800}{1.987 T} \right) \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(b) Steam and Oxygen	McGillivray (1)	$\frac{0.4195 \frac{P_{st}}{1000} \exp \left(\frac{-6432}{T} \right)}{1 + 2.48E-7 \frac{P_{st}}{1000} \exp \left(\frac{5327}{T} \right)} + 10.95 \exp \left(\frac{-8077}{T} \right) \frac{\text{kg O}_2}{\text{m}^2 \cdot \text{s}}$
(c) Dry, T < 300°C	Trimble	$10^{\left(7.19 - \frac{3732.0}{T} \right)} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(d) Dry, T > 300°C	Pearce (2)	$10^{\left(28.381 - 7 \log T - \frac{4638.2}{T} \right)} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(e) Oxygen Free	Pearce (2)	$10^{\left[4.33 - \frac{2144}{T} + 0.5 \log \left(\frac{P_{st}}{1000} \right) \right]} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(f) 100% RH, T < 100°C	Pearce (2)	$10^{\left(8.333 - \frac{3730}{T} \right)} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(g) ≤ 75% RH, T < 100°C	Ritchie (2, 5)	$10^{\left(13.8808 - \frac{5.7696E3}{T} \right)} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(h) Moist, T > 465 K	Pearce (2)	$10^{\left[6.1931 - \frac{2963}{T} + 0.3 \log \left(\frac{P_{st}}{1000} \right) \right]} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$
(i) Moist, T < 465 K	Pearce (2)	$10^{\left[10.566 - \frac{4990}{T} + 0.3 \log \left(\frac{P_{st}}{1000} \right) \right]} \frac{\text{mg O}_2}{\text{cm}^2 \cdot \text{hr}}$

Notes:

- (1) Part of the first set of rate laws.
- (2) Part of the alternate set of rate laws.
- (3) Except for McGillivray's correlation, units are (mg O₂ / cm² hr).
- (4) Temperatures are in degrees K and pressures are in Pa. Temperatures are bounded by 273.15 K and 1273.15 K.
- (5) For RH between 75% and 100%, HANSF interpolates between the Pearce and Ritchie correlations.

Figure 3-9: Oxidation Rate Law Logic.

BM98n029.CDR 3-3-99

First, based on the individual fuel/scrap heat sink temperature and the condition in the surrounding gas (dry, wet, oxygen-free, oxygenated, etc.), the oxidation rate law is evaluated for the dry surface and for the wet surface. The rate law is multiplied by the appropriate area and multiplier to determine the oxygen uptake rate by the uranium, the hydride, and the dehydrided hydride ($W_{O_2,U,i}$, $W_{O_2,hyd,i}$, and $W_{O_2,dehyd,i}$) for each heat sink surface- i . The total oxygen uptake rate ($W_{O_2,i} = W_{O_2,U,i} + W_{O_2,hyd,i} + W_{O_2,dehyd,i}$) and its fractional contributors ($f_{O_2,U,i} = W_{O_2,U,i} / W_{O_2,i}$, $f_{O_2,hyd,i} = W_{O_2,hyd,i} / W_{O_2,i}$, $f_{O_2,dehyd,i} = W_{O_2,dehyd,i} / W_{O_2,i}$) are noted. Also, the fraction of oxygen uptake by dry surface, $f_{unc,i}$, is determined.

Next, the oxygen reaction rate is limited by available oxygen and steam mass. Since some oxygen reacts with hydrides to form water vapor (reaction 3 above), the actual oxygen requirement is greater than the oxygen uptake. The oxygen requirement for each heat sink surface is given by:

$$W'_{O_2,i} = f_{unc,i} \{ W_{O_2,U,i} + (1.75 (1 - FO2HYH2) + FO2HYH2) W_{O_2,hyd,i} + W_{O_2,dehyd,i} \} \quad (3-4)$$

Where again, FO2HYH2 is a user parameter for the reaction path. The oxygen requirement is summed over all heat sink surfaces:

$$W_{O_2}^{(1)} = \sum W_{O_2,i}^{(1)} \quad (3-5a)$$

and

$$W_{O_2} = \sum W_{O_2,i} \quad (3-5b)$$

On the other hand, if all oxygen demand on the uncovered surface is to be met by steam, the steam consumption rate is given by

$$W'_{st,i} = \frac{2 M_{W_{H_2O}}}{M_{W_{O_2}}} f_{unc,i} W_{O_2,i} \quad (3-5c)$$

Likewise, the water requirement for each heat sink is given by

$$W'_{w,i} = f_{cov,i} \frac{2 M_{w_{H_2O}}}{M_{w_{O_2}}} W_{O_2,i} \quad (3-5d)$$

where $f_{cov,i} = 1 - f_{unc,i}$. Of course, it is limited by available water;

$$W'_{w,i} = \min \left(W'_{w,i}, \frac{M_{w_i}}{2 \Delta t} \right) \quad (3-5e)$$

The water consumption rate on the covered fuel surface per each kg of demanded oxygen weight gain is given by

$$f_{rx,w,i} = \frac{W'_{w,i}}{W'_{O_2,i}} \quad (3-5f)$$

Then, the actual oxygen consumption rate for each kg of demanded oxygen weight gain is determined by:

$$f_{rx,O_2} = \frac{W'_{O_2}}{W_{O_2}} \min \left(1, \frac{M_{O_2}}{W'_{O_2} 2 \Delta t} \right) \quad (3-6)$$

where M_{O_2} is the mass of oxygen and Δt is the time step. The factor "2" in the denominator is introduced for under-relaxation.

The remaining oxygen uptake on dry surface has to come from steam. That is, the steam consumption rate per each kg of demanded oxygen weight gain is given by

$$f_{rx,H_2O} = 2 \frac{M_{w_{H_2O}}}{M_{w_{O_2}}} \frac{W'_{st}}{W_{O_2}} \left(1 - \min \left(1, \frac{M_{O_2}}{W'_{O_2} 2 \Delta t} \right) \right) \quad (3-7)$$

where f_{rx,H_2O} is the consumption rate of water vapor for each kg of oxygen rate demanded by the correlation, and $M_{w_{H_2O}}$ and $M_{w_{O_2}}$ are molecular weight of water and oxygen, respectively. The corresponding steam consumption rate is given by:

$$W_{H_2O} = f_{rx,H_2O} W_{O_2} \quad (3-8)$$

Of course, the steam consumption rate is limited by available steam. That is,

$$f_{rx,H2O} = f_{rx,H2O} \min \left(1, \frac{M_{H2O}}{W_{H2O} 2 \Delta t} \right) \quad (3-9)$$

Now, each individual heat sink surfaces are revisited and the actual rate terms are evaluated as follows:

- Oxygen consumption rate: $f_{rx,O2} W_{O2,i}$
- Water vapor consumption rate: $f_{rx,H2O} W_{O2,i}$
- Liquid water consumption rate: $f_{rx,w,i} W_{O2,i}$
- Water vapor production rate due to oxidation of hydride:

$$\frac{3}{2} \frac{Mw_{H2O}}{Mw_{O2}} f_{O2,hyd,i} f_{rx,O2} W_{O2,i} (1 - FO2HYH2)$$

- Hydrogen production rate:

$$\begin{aligned} & \frac{Mw_{H2}}{Mw_{H2O}} (f_{rx,H2O} + f_{rx,w,i}) W_{O2,i} \left(f_{O2,U,i} + \frac{3.5}{2} f_{O2,hyd,i} + f_{O2,dehyd,i} \right) \\ & + \frac{3}{2} \frac{Mw_{H2}}{Mw_{O2}} f_{rx,O2} W_{O2,i} f_{O2,hyd,i} FO2HYH2 \end{aligned}$$

- Reaction energy deposited on the surface:

$$\begin{aligned} & 3.4 \cdot 10^7 f_{rx,O2} W_{O2,i} (f_{O2,U,i} + f_{O2,dehyd,i}) \\ & + 3.0 \cdot 10^7 f_{rx,O2} W_{O2,i} f_{O2,hyd,i} FO2HYH2 \\ & + 2.4 \cdot 10^7 f_{rx,O2} W_{O2,i} f_{O2,hyd,i} (1 - FO2HYH2) / 1.75 \\ & + 1.67 \cdot 10^7 \left(\frac{Mw_{O2}}{Mw_{H2O}} / 2 \right) (f_{rx,H2O} + f_{rx,w,i}) W_{O2,i} (f_{O2,U,i} + f_{O2,dehyd,i}) \\ & + 1.37 \cdot 10^7 \left(\frac{Mw_{O2}}{Mw_{H2O}} / 2 \right) (f_{rx,H2O} + f_{rx,w,i}) W_{O2,i} f_{O2,hyd,i} \end{aligned}$$

- UO_2 production rate:

$$270 \left(f_{\text{rx},\text{O}_2} \frac{W_{\text{O}_2,i}}{Mw_{\text{O}_2}} + (f_{\text{rx},\text{H}_2\text{O}} + f_{\text{rx},\text{w},i}) \frac{W_{\text{O}_2,i}}{2 Mw_{\text{H}_2\text{O}}} \right) \quad |$$

- U (metal) depletion rate:

$$238 \left(f_{\text{O}_2,\text{U},i} f_{\text{rx},\text{O}_2} \frac{W_{\text{O}_2,i}}{Mw_{\text{O}_2}} + f_{\text{O}_2,\text{U},i} (f_{\text{rx},\text{H}_2\text{O}} + f_{\text{rx},\text{w},i}) \frac{W_{\text{O}_2,i}}{2 Mw_{\text{H}_2\text{O}}} \right) \quad |$$

- Hydride depletion rate:

$$241 \left(f_{\text{O}_2,\text{hyd},i} f_{\text{rx},\text{O}_2} \frac{W_{\text{O}_2,i}}{Mw_{\text{O}_2}} + f_{\text{O}_2,\text{hyd},i} (f_{\text{rx},\text{H}_2\text{O}} + f_{\text{rx},\text{w},i}) \frac{W_{\text{O}_2,i}}{2 Mw_{\text{H}_2\text{O}}} \right) \quad |$$

- Dehydrided hydride depletion rate:

$$238 \left(f_{\text{O}_2,\text{dehyd},i} f_{\text{rx},\text{O}_2} \frac{W_{\text{O}_2,i}}{Mw_{\text{O}_2}} + f_{\text{O}_2,\text{dehyd},i} (f_{\text{rx},\text{H}_2\text{O}} + f_{\text{rx},\text{w},i}) \frac{W_{\text{O}_2,i}}{2 Mw_{\text{H}_2\text{O}}} \right) \quad |$$

Currently, the energy of the reactant gas consumed during the reaction is removed from the gas space and the energy of the product gas corresponding to the heat sink surface temperature is added to the gas space. However, these gas energies are not considered in the energy balance of the heat sink. Normally, the heat of reaction at a given temperature, usually 25°C, is tabulated in the literature. Therefore, to be strictly correct, any excess enthalpy of the reactant gas above 25°C should be added to the heat sink, and the energy needed to bring the temperature of the product gas from 25°C to the heat sink temperature should be subtracted from the energy of the heat sink.

3.4 Hydriding / Dehydriding

Hydride formation in the presence of hydrogen gas in an MCO or hydride decomposition in its absence is represented by the reaction:

The direction of the reaction depends on the hydrogen pressure relative to equilibrium. Unfortunately, the only data available for this process are for nearly-pure hydrogen systems. The best correlation available is that of [Bloch and Mintz, 1981]:

$$u_g (P_{H_2}, T) = K_{eq} \left[\left(\frac{P_{H_2}}{P_d} \right)^{\frac{n}{2}} \left(\frac{1 + K_m P_d^{1/2}}{1 + K_m P_{H_2}^{1/2}} \right)^n - \left(\frac{P_d}{P_{H_2}} \right)^{\frac{m}{2}} \right] \quad (3-10a)$$

$$K_{eq} = K_f [K_m P_d^{1/2} / (1 + K_m P_d^{1/2})]^n \quad (3-10b)$$

$$\ln [P_d \text{ (atm)}] = 16.2 - 11050 / T \quad (3-10c)$$

$$K_f \text{ (microns/min)} = (89.9E3) \exp (-7600 / 1.987 T) \quad (3-10d)$$

$$K_m \text{ (torr}^{-1/2}) = (9.25E-4) \exp (3100 / 1.987 T) \quad (3-10e)$$

where $u_g (P_{H_2}, T)$ is the linear velocity of the reaction front in microns/minutes; P_{H_2} is the working pressure in torr; P_d is the hydrogen equilibrium disassociation pressure, which must be converted to torr for use; $n = 2$; $m = 1$; and T is in Kelvin.

The Bloch and Mintz correlation predicts hydriding, or $u_g > 0$, when $P_{H_2} > P_d$ and predicts dehydriding, or $u_g < 0$, when $P_{H_2} < P_d$. Use of this correlation probably overpredicts reaction rates in the presence of non-condensable gases and in the concurrent presence of oxidation. The code accounts for such uncertainties by providing multipliers on both the hydriding and dehydriding rates.

The rate laws for oxidation of uranium apply to hydride as well. However, significantly higher reaction areas of hydride compared to pure uranium metal have to be taken into consideration: about 0.5 m² per gram is the typical surface area density of the initially created hydride particles. However, the surface area density can increase up to a factor of two or three as it goes through dehydriding/hydrating cycles. A single input constant particle size is used to characterize the area through the standard relation

$$A = \frac{M}{\rho} \frac{6}{d} \quad (3-11)$$

where M = hydride or dehydrided metal mass,

ρ = particle density, and

d = particle diameter.

Hydride oxidation area can be handled in one of three ways, depending on user choice. The first is to calculate the area mechanistically using equation (3-11). The user can also choose to keep the area constant indefinitely, or keep the area constant while there is dehydrided metal mass, but zero once all the dehydrided metal mass is consumed.

3.5 Uranium Oxide Hydrate Decomposition

3.5.1 Assumptions

Uranium oxide hydrates are assumed to exist as $\text{UO}_3 \cdot x\text{H}_2\text{O}$ and to decompose serially from $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ to UO_3 . The hydrated fraction of sludge, the initial stoichiometry, and stoichiometry of intermediate hydrates are user-specified. Up to three decomposition steps are allowed, for example:

The initial mass of hydrate is specified using two parameters: f_o is the fraction of sludge that is hydrated, and x_o is the stoichiometry number of the hydrate (ratio of H_2O / U). If M_{sl} is the mass of hydrate on a fuel element or scrap node surface, then the hydrate mass and water mass are given by

$$M_{hy} = f_o \cdot M_{sl} \quad (3-12)$$

$$M_{why} = \frac{18x_o}{286 + 18x_o} M_{hy} \quad (3-13)$$

At any time, the water mass fraction of the hydrated material is given by

$$f_w = \frac{M_{why}}{M_{hy}} \quad (3-14)$$

and its stoichiometry number is

$$x = \frac{286}{18} \frac{f_w}{1 - f_w} \quad (3-15)$$

3.5.2 Equilibrium and Decomposition Laws

Equilibrium pressure for the hydrates is given for three stages of decomposition.

$$\ln P_{eq} = A_1 + \frac{B_1}{T} \quad x_2 \leq x \leq 2 \quad (3-16a)$$

$$\ln P_{eq} = A_2 + \frac{B_2}{T} \quad x_3 \leq x < x_2 \quad (3-16b)$$

$$\ln P_{eq} = A_3 + \frac{B_3}{T} \quad 0 \leq x < x_3 \quad (3-16c)$$

where A_i and B_i are input parameters and $0 \leq x_3 \leq x_2 < 2$ are also input parameters.

Decomposition can occur whenever

$$P_v < P_{eq} \quad (3-17)$$

where P_v is the ambient steam pressure. The rate of decomposition is given by

$$\frac{df_w}{dt} = -K(T) (f_w - f_w^o) \quad (3-18)$$

where f_w^o is the target water mass fraction of the intermediate decomposition step. Decomposition rate laws correspond to the decomposition steps:

$$\ln K(T) = A_{K1} + \frac{B_{K1}}{T} \quad x_2 \leq x \leq 2 \quad (3-19a)$$

$$\ln K(T) = A_{K2} + \frac{B_{K2}}{T} \quad x_3 \leq x < x_2 \quad (3-19b)$$

$$\ln K(T) = A_{K3} + \frac{B_{K3}}{T} \quad 0 \leq x < x_3 \quad (3-19c)$$

where A_{Ki} and B_{Ki} are input parameters. Note that by setting A_{Ki} , B_{Ki} , and x_i equal, one or two steps in decomposition are simulated. It should be noted that the above exponential rate law implies that the mass of one stage never truly goes zero. Therefore, when one stage is nearly complete (99%), the next stage is allowed to start.

An implicit version of the rate law definition using the end-of-timestep value is best:

$$\frac{F_w - F_w^o}{\Delta t} = -K(T) F_w \quad (3-20a)$$

$$F_w = \frac{F_w^o}{1 + K(T) \Delta t} \quad (3-20b)$$

$$\left(\frac{dF_w}{dt} \right)_{im} = \left(\frac{dF_w}{dt} \right)_{ex} (1 + K(T) \Delta t)^{-1} \quad (3-20c)$$

where "im" and "ex" stand for implicit and explicit, respectively. Therefore, the mass rate of dehydration is

$$\frac{dM_{\text{why}}}{dt} = -K(T) (M_{\text{why}} - M_{\text{why}}^*) (1 + K(T) \Delta t)^{-1} \quad (3-21)$$

where M_{why}^* is the target water mass.

3.5.3 Decomposition Limitations

A mass transfer limitation may exist for low water vapor pressures near the equilibrium value. The diffusion controlled mass transfer rate is calculated from the Chilton-Colburn analogy of equations (2-18a), (2-18b), and (2-18c).

Because many surfaces may have hydrates and be at different temperatures, but a single gas space temperature and water vapor pressure is common to those surfaces, it is possible that for some cooler surfaces $P_{\text{eq}} < P_v$, so no decomposition occurs; and for some hotter surfaces $P_{\text{eq}} > P_v$, so decomposition occurs. In fact, the rate of decomposition of hotter surfaces may be great enough that decomposition of cooler surfaces, allowed at the beginning of a timestep, would stop in the middle of a timestep. Using the ideal gas law, the extrapolated water vapor pressure after decomposition is given by

$$P_{\text{ex}} = P_v + \frac{\Delta n RT}{V} \quad (3-22a)$$

$$\Delta n = \frac{1}{18} \sum \left(\frac{dM_{\text{why}}}{dt} \right) \Delta t \quad (3-22b)$$

where T and V are the gas space temperature and volume, respectively, and R is the ideal gas constant. For any surface where

$$P_v < P_{\text{eq}} < P_{\text{ex}} \quad (3-23)$$

decomposition will only occur through a portion of a timestep.

An approximate way to limit "overshoot" of cooler surfaces is to multiply the rate law by the fraction of a timestep decomposition can occur, given by

$$f_{\text{dec}} = \frac{P_{\text{eq}} - P_v}{P_{\text{ex}} - P_v} \quad (3-24)$$

This is valid because the contribution of cooler surfaces to P_{ex} is small, hence, the value of P_{ex} is relatively unchanged by a limitation on their decomposition.

3.6 Heat Transfer in the Fuel Basket

Decay and oxidation heat generated in the fuel elements are normally transferred radially outward via radiation and micro-convection to the MCO wall. From the MCO wall, heat is either removed by the circulating water jacket, or is radiated and convected to the cask wall, which is cooled by natural convection outside. If a gas is circulating through the MCO, some heat would be diverted to the gas. In the code, the detailed radiation heat transfer between individual fuel elements and with the MCO wall is considered. In addition, heat transfer via micro-convection between adjacent fuel elements and MCO wall is considered. Global natural circulation inside MCO is assumed to be negligible. Although radiative heat loss from one end of fuel elements to the MCO lid or floor is considered, such heat transfer between tiers is neglected. Axial conduction along fuel elements is assumed sufficiently large to warrant no appreciable axial temperature gradient.

3.6.1 Radiation Heat Transfer

Radiation heat transfer is a dominant mechanism for heat removal from the MCO. The model represents radiation from the exterior of the cask (or vault) to the ambient gas, and from

one heat sink to another within the MCO. For situations where planar geometry is a good approximation, radiation can be expressed in the form of a transport coefficient:

- Between the cask (vault) wall heat sink and the ambient gas,

$$h_{\text{rad}} = \frac{\sigma (T_g^2 + T_w^2) (T_g + T_w)}{\left(\frac{1}{\epsilon_g} + \frac{1}{\epsilon_w} - 1 \right)} \quad (3-25)$$

where σ = Stefan-Boltzmann constant,

$$= 5.7 \times 10^{-8} \text{ W/(m}^2\text{K}^4\text{)},$$

T_g = gas temperature,

T_w = cask (vault) wall temperature,

ϵ_g = emissivity of gas (= 0.60), and

ϵ_w = emissivity of wall (user-specified).

- Between inner and outer fuel elements, between the MCO wall and the cask wall, and between fuel elements and the floor/lid,

$$h_{\text{rad}} = \frac{F \sigma (T_{w_1}^2 + T_{w_2}^2) (T_{w_1} + T_{w_2})}{\left(\frac{1}{\epsilon_{w_1}} + \frac{1}{\epsilon_{w_2}} - 1 \right)} \quad (3-26)$$

where F = view factor. The following are user-specified: (1) emissivities for the fuel, the MCO, and the cask walls, and (2) the view factor between the outer fuel elements and the MCO wall.

The view factor between the inner and outer elements is assumed to be one; so is the view factor between the MCO wall and the cask wall.

For the radiation heat transfer between each fuel element and the floor/lid, the view factor is taken to be the volume fraction of the particular fuel element to the total fuel volume in the basket. Of course, the floor/lid surface area is used in conjunction with the view factor.

For the pin-by-pin model, input values for view factors between outer fuel elements and the MCO wall inside the 30° base cell sector were determined using the first principles view

factor definition. Table 3-3 shows the resulting view factor matrix. View factors for direct radiation from an in-sector donor to an out-of-sector receiver are incorporated by effectively adding that radiant heat to the in-sector mirror-image of the actual receiver node. For example (refer to Figure 3-7), the view factor which accounts for "shine" from heat sink 6 that passes between heat sinks 4 and 8 is simply added to the view factor for radiation from 6 to 8. In this way, all direct radiation paths are accounted for. The radiation heat transfer rates are calculated from radiosities. First, the radiosity for each heat sink is determined by solving the system of linear equations

$$B_j = \epsilon_j \sigma T_j^4 + \rho_j \left[\sum_{i=1}^N B_i F_{j-i} \right] \quad (3-27)$$

where B_j = radiosity of heat sink - j (the rate at which radiant heat leaves a surface per unit area),

ρ_j = reflectance,

ϵ_j = emissivity of surface j, and

F_{j-1} = view factor from surface j to i.

Once the radiosity is known, the net heat loss due to radiation can be obtained by

$$Q_j = A_j \left[\frac{\epsilon_j \sigma T_j^4 - (1 - \rho_j) B_j}{\rho_j} \right] \quad (3-28)$$

Figure 3-10 shows the flowchart of radiation heat transfer calculation in the fuel basket.

3.6.2 Micro-Convection Heat Transfer

In the absence of global connective heat transfer inside the sealed MCO, micro-convection heat transfer between adjacent fuel rods and the MCO wall and inside the gap between the MCO and the cask (vault) wall is considered. For the case of an enclosed vertical volume, the natural convection Nusselt number is related to the Rayleigh number by:

Table 3-3: View Factors For Pin-By-Pin Model

	To: Insert ⁽¹⁾	4 ⁽²⁾	6	8	10	12	14	16	17 (MCO Wall)
From: Insert ⁽¹⁾	0	0.926	0.074	0	0	0	0	0	0
4 ⁽²⁾	0.175	0.316	0.306	0.181	0.028	0	0	0	0
6	0.014	0.306	0.028	0.306	0.306	0.028	0.014	0	0
8	0	0.181	0.306	0	0.334	0.153	0	0.028	0
10	0	0.014	0.153	0.167	0.167	0.153	0.153	0.167	0.028
12	0	0	0.028	0.153	0.306	0	0.028	0.306	0.181
14	0	0	0.014	0	0.306	0.028	0	0.306	0.348
16	0	0	0	0.014	0.167	0.153	0.153	0.049	0.466
17 (MCO Wall)	0	0	0	0	0.035	0.115	0.22	0.59	0.04

⁽¹⁾ For example, view factor from Insert to Heat Sink 4 is 0.926.

⁽²⁾ Heat sink number from Figure 3-7.

Figure 3-10:
Flowchart for Radiation Heat Transfer Calculation
Between Fuel Elements, the MCO Wall, and the Insert.

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$$\text{Nu} = \max \left(1.0, 0.364 \text{ Ra}^{1/4} \left(\frac{x_{\text{gap}}}{L} \right)^{1/4} \right) \quad (3-29)$$

where x_{gap} is the gap distance and L is the height of the enclosure. The distance between the inner and outer fuel elements is 0.003 m. Nominal distance between the outer elements and the MCO wall are summarized in Table 3-4. The lower limit of 1.0 in equation (3-29) represents the conduction heat transfer across the interstitial gas. Once the heat transfer coefficient is determined, the actual heat transfer rate from one heat sink to another is given by:

$$Q_{\text{conv}} = F_{i-j} h_{\text{conv}} A_i (T_i - T_j) \quad (3-30)$$

where F_{i-j} is the radiation view factor in Table 3-3.

Table 3-4: Conduction Distance (m) - Pin-By-Pin Model

	To: Insert (1)	4 (2)	6	8	10	12	14	16	17 (MCO Wall)
From: Insert (1)	0	0.018	0	0	0	0	0	0	0
4 (2)	0.018	0	0.021	0.021	0.073	0	0	0	0
6	0	0.021	0	0.021	0.021	0.073	0.073	0	0
8	0	0.021	0.021	0	0.021	0.021	0	0.073	0
10	0	0.073	0.021	0.021	0	0.021	0.021	0.021	0.083
12	0	0	0.073	0.021	0.021	0	0.073	0.021	0.058
14	0	0	0.073	0	0.021	0.073	0	0.021	0.026
16	0	0	0	0.073	0.021	0.021	0.021	0	0.016
17 (MCO Wall)	0	0	0	0	0.083	0.058	0.026	0.016	0

(1) For example, distance from Insert to Heat Sink 4 is 0.018 m.
 (2) Heat sink number from Figure 3-7.

3.6.3 Diversion Heat Transfer to Gas

Note that the micro-convection heat transfer described above bypasses the interstitial gas. Actually, some heat transfer would be diverted to heat the interstitial gas. To determine the amount of heat being diverted, expected local mean gas temperatures are themselves averaged and then compared with the MCO gas node bulk temperature. A fraction of heat sink-to-heat sink heat transfer is then diverted to (or from) the gas node to equilibrate the two temperatures. Of course, this diversion heat transfer rate is bounded by the micro-convection heat transfer coefficient. Because the heat capacity of the gas in the MCO is small, only a minute amount of heat needs to be so diverted. If a cold gas circulates through the MCO, it is possible that this diversion heat can exceed the micro-convection heat transfer rate, leading to general cooling of the fuel by circulating gas.

First, micro-convection heat transfer is calculated between every two adjacent heat sinks. Then, a fraction of the heat transfer rate is diverted to heat the interstitial gas so that the gas temperature can realistically follow the heat sink temperatures. The total diverted heat in a region is determined by,

$$AHTSUM = \sum F_{i-j} h_{conv} A_i \quad (3-31a)$$

$$ATSUM = \sum A_{ii} T_{ii} + A_{2i} T_{2i} \quad (3-31b)$$

$$ASUM = \sum A_{ii} + A_{2i} \quad (3-31c)$$

where the summation is over every adjacent heat sink pairs. The average heat sink temperature is given by,

$$T_{avg} = \frac{ATSUM}{ASUM} \quad (3-32)$$

The total heat to be diverted is given by

$$Q_{\text{divert}} = \min \left(\text{AHTSUM}, M_g \frac{c_{pg} / \lambda_{\text{relax}}}{\Delta t} \right) (T_{\text{avg}} - T_g) \quad (3-33)$$

where M_g = Mass of gas in the region,
 c_{pg} = Specific heat of gas,
 λ_{relax} = Relaxation factor (number of fuel/scrap baskets in the gas region),
 Δt = Time step, and
 T_g = Gas temperature in the region.

Lastly, every adjacent heat sink pair is visited again to apportion the total diverted heat among all participating heat sink surfaces weighted by area. That is,

$$Q_{\text{divert},j} = \frac{A_j}{\text{ASUM}} Q_{\text{divert}} \quad (3-34)$$

The diversion heat transfer model works well when the temperature gradient in a fuel/scrap basket is moderate. However, during a run-away, because of the bias of the hot spot in the average fuel temperature, the diversion heat is taken out continually from the cold fuel, even when it is freezing. A model parameter, IDIVRT, was provided to give the user an option to suppress individual heat sink diversion heat transfer under certain conditions. The available options for IDIVRT flag are as follows:

IDIVRT = 0, no diversion heat transfer calculation,
 = 1, normal diversion heat transfer calculation,
 = 2, suppress the individual diversion when:
 $Q_{\text{divert}} > 0$ but $T_{\text{fuel},i} < T_{\text{gas}}$
 or
 $Q_{\text{divert}} < 0$ but $T_{\text{fuel},i} > T_{\text{gas}}$
 = 3, suppress the individual diversion when:
 $Q_{\text{divert}} > 0$ but $T_{\text{fuel}} < T_{\text{gas}}$.

3.7 Heat Transfer in the Scrap Basket

3.7.1 Effective Thermal Conductivity in a Rubble Bed

For the scrap basket, effective thermal conductivity in a rubble bed is used to characterize the thermal resistance inside the basket. This effective thermal conductivity takes into account the radiation between scrap pieces and the conduction through the fuel scraps as well as through the interstitial gas. It is given by,

$$k_{\text{eff}} = 1.8 k_g \left(\ln \left(\frac{k_s}{k_g} \right) - 1 \right) + 4 \sigma \epsilon x_{\text{eff}} T_s^3 \quad (3-35)$$

$$\text{where } x_{\text{eff}} = \frac{x_D \left(1 + \frac{\lambda}{\epsilon} \right)}{1 - \lambda} \quad (3-36)$$

$$\lambda = 1 - 1.21 (1 - \text{porosity})^{0.67},$$

$$k_g = \text{Thermal conductivity of the interstitial gas,}$$

$$k_s = \text{Thermal conductivity of the fuel scrap,}$$

$$\sigma = \text{Stefan-Boltzmann constant,}$$

$$\epsilon = \text{Emissivity of fuel scrap (user-specified), and}$$

$$x_D = \text{Characteristic diameter of the scrap.}$$

3.7.2 Nodalization of Scrap Basket and Treatment of "Fin"

Copper-lined spokes and the scrap basket wall act as 'fins' to promote dissipation of reaction and decay power generated by fuel scrap in the interior (Figure 3-8). In the following discussion, "radial fin" refers to the copper-lined spokes and "peripheral fin" refers to the copper-lined basket wall.

The analytical solution for the temperature profile in a circular sector of a volumetric heat generating medium where the boundary is kept at a uniform temperature shows the maximum

temperature occurs not at the center of the circle, but at some distance 'a' from the center. Therefore, for the interior region (i.e., inside 'a'), the "radial fin" becomes the closest heat sink and the dominant heat transfer direction is azimuthal. On the other hand, for the exterior region (i.e., outside 'a'), the "peripheral fin" provides the closest heat sink and the dominant heat transfer direction is radially outward.

Consider a sector of a circle whose boundaries are kept at uniform temperature $T = 0$. The interior of the sector is heated uniformly and volumetrically at the rate $\dot{Q}$ (in W/m^3). Then in steady-state, the conduction equation for the temperature field is

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\dot{Q}}{k} = 0 \quad (3-37)$$

subject to the boundary conditions

$$T = 0 \quad \text{at} \quad \theta = 0 \quad (3-38a)$$

$$T = 0 \quad \text{at} \quad \theta = \theta_0 \quad (3-38b)$$

$$T = 0 \quad \text{at} \quad r = R \quad (3-38c)$$

$$\frac{\partial T}{\partial r} = 0 \quad \text{at} \quad r = 0 \quad (3-38d)$$

where k is the thermal conductivity of the sector material and θ_0 is the angle between the sector's radii boundaries, such that the angular coordinate $0 < \theta < \theta_0$. A solution for the temperature is:

$$\frac{T_{CL} \pi k}{2 \dot{Q} R^2} \sim \frac{2}{\left(\frac{\pi}{\theta_0} \right)^2 - 4} \left[\left(\frac{r}{R} \right)^2 - \left(\frac{r}{R} \right)^{\frac{\pi}{\theta_0}} \right] \quad (3-39)$$

where T_{CL} denotes the centerline temperature profile. Differentiating this expression with respect to r/R and setting the result equal to zero, we find that the temperature is a maximum at

$$\frac{a}{R} \sim \left(\frac{2 \theta_0}{\pi} \right)^{\frac{\theta_0}{\pi - 2 \theta_0}} \quad (3-40)$$

For $\theta_0 = 60^\circ$, $a/R = 0.67$.

A one-dimensional, porous medium heat transfer model can be used separately for the exterior and interior regions to mimic the two-dimensional heat transfer. For the exterior region, azimuthal heat transfer is neglected and only radial heat transfer is considered. For the interior region, each annular ring is azimuthally sub-divided into several heat sinks which are connected together to transfer heat in the azimuthal direction. Heat transfer between the adjacent rings is neglected. Note that this simple one-dimensional model is always conservative as it neglects minor heat transfer paths.

Each heat sink forms the basic unit of the scrap basket for distributed quantities, such as the amount of uranium oxide, hydride, water, etc. Temperature is tracked in each heat sink node. The inner surface temperature of each heat sink is used to evaluate the temperature dependent rates for oxidation, evaporation, dehydration, etc.

Temperature continuity across the adjacent heat sinks is enforced by calculating an appropriate surface heat flux; i.e., the boundary temperatures of two adjacent heat sinks overlap. Therefore, the heat transfer rate across the interface, Q_f , is given by,

$$Q_f = A_f \frac{k_i + k_{i-1}}{2} \frac{(T_{i-1}(N-1) - T_i(2))}{\Delta x_{i-1} + \Delta x_i} \quad (3-41)$$

where A_f is the heat transfer area, k is the thermal conductivity, $T_i ()$ is the node temperature for heat sink "i", and Δx_i is the node thickness for heat sink "i". Temperature continuity dictates that $T_{i-1}(N) = T_i(1)$; the outer surface temperature of heat sink "i - 1" equals the inner surface temperature of heat sink "i". Note, the heat transfer rate uses the average thermal conductivity and the appropriate distance between nodes. The heat transfer rate Q_f is applied as the surface sink term for the outer surface of heat sink "i - 1" and as the surface source term for the inner surface of heat sink "i".

The fin is a separate planar heat sink. The fin heat sink is flush with the boundary heat sinks of the scrap sector; the inner surface node of the fin coincides with the outer surface node of the boundary scrap heat sinks. To determine the surface heat flux needed to maintain the uniform temperature, solve for the next-time-step interface temperature in

$$(M c_p)_{fin} \frac{T^* - T_{fin}(1)}{\Delta t} = \sum_{i=1}^N k_i A_i \frac{T_i(N-1) - T^*}{\Delta x_i} - A_{ext} h_{rad} (T^* - T_{mco}) - A_{ext} h_{conv} (T^* - T_{mco}) \quad (3-42)$$

where N is the number of boundary heat sinks, T^* is the next-time-step interface temperature, A_i is the boundary heat sink surface area for heat sink "i", and A_{ext} is the external boundary surface area. After rearranging, we obtain,

$$T^* = \frac{(M c_p)_{fin} \frac{T_{fin}(1)}{\Delta t} + \sum_{i=1}^N k_i A_i \frac{T_i(N-1)}{\Delta x_i} + A_{ext} h_{rad} T_{mco} + A_{ext} h_{conv} T_{mco}}{\frac{(M c_p)_{fin}}{\Delta t} + \sum_{i=1}^N k_i \frac{A_i}{\Delta x_i} + A_{ext} h_{rad} + A_{ext} h_{conv}} \quad (3-43)$$

Thus, each interface heat transfer rate to be taken out from the boundary surfaces and added to the fin surface is given by

$$Q_{fi} = k_i A_i \frac{T_i(N-1) - T^*}{\Delta x_i} \quad (3-44)$$

The radiative heat transfer rate from the fin to the MCO wall is given by

$$Q_{rad} = h_{rad} A_{ext} (T^* - T_{mco}) \quad (3-45)$$

Lastly, the micro-convection heat transfer rate from the fin to the MCO wall is given by

$$Q_{conv} = h_{conv} A_{ext} (T^* - T_{mco}) \quad (3-46)$$

Figure 3-11 shows the flowchart for heat transfer calculation in the scrap basket.

3.7.3 Diversion Heat Transfer to Gas in Scrap Basket

In order to determine the diverted heat, the effective thermal conductivity is used to estimate the micro-convection heat transfer coefficient to the gas. That is,

Figure 3-11: Flowchart for Heat Transfer Calculation in the Scrap Basket.

$$h_{\text{micro}} = \frac{k_{\text{eff}}}{x_D/2} \quad (3-47)$$

The actual exposed area of the scrap is used to determine the diverted heat:

$$A_{\text{eff}} = \frac{6 (1 - \text{porosity}) V}{x_D} \quad (3-48)$$

where V is the bulk volume of the scrap node.

Heat diversion to the interstitial gas is done in a similar way as in the fuel basket (see Section 3.6.3).

3.8 Evaporation and Condensation

Residual water evaporation in the MCO, and subsequent condensation and revaporization, is modeled using standard mass transfer correlations. For diffusion controlled mass transfer, the evaporation ("negative" condensation) rate, $\dot{m}$, is calculated from the Chilton-Colburn analogy of equations (2-28a), (2-28b), and (2-28c).

Basically, the evaporation rate is nearly proportional to the difference between the mass fraction of saturated steam at the surface temperature and the mass fraction of steam in the free stream. In the current formulation, the evaporation rate is linearized with respect to the steam partial pressure difference between at the surface and in the free stream.

If $P_{\text{sat}}(T_w)$ is greater than P, bulk boiling occurs and its rate would not be diffusion controlled. Likewise, for nearly pure steam ($P_{\text{st}} \approx P$), condensation/evaporation is not limited by mass diffusion. For either case, the transport rate is subject to the Langmuir limitation, particularly for flashing/boiling which may occur under rapid depressurization, such as during a vacuum drying process. The Langmuir equation limits how rapidly water molecules can be removed from the surface during boiling and how rapidly water molecules can condense on the surface in the absence of non-condensibles. Evaporation/condensation can be modeled as

occurring across two layers: the Langmuir layer, and the mass diffusion layer. By considering the Langmuir layer between the heat sink surface and the mass diffusion layer in the free stream, the transition between the mass diffusion controlled rate and Langmuir limited rate can be calculated without numerical difficulties.

In the presence of non-condensibles, the evaporation rate is normally controlled by mass diffusion and the resistance in the Langmuir layer is minimal; that is, $P_{st,I} \approx P_{sat}(T_w)$, where $P_{st,I}$ is the vapor pressure at the interface between layers, and $P_{sat}(T_w)$ is the saturation pressure at the wall temperature. However, when boiling occurs, $P_{sat}(T_w) > P$, the bulk or free stream vapor pressure and the resistance in the Langmuir layer increases to limit evaporation such that $P_{sat}(T_w) \geq P \geq P_{st,I}$. The first equality occurs when the evaporation rate is very low, and all resistance is by diffusion (when non-condensibles are present). Likewise, in the absence of non-condensibles, the mass diffusion layer disappears completely and the Langmuir layer solely controls the mass transfer, and the second inequality approaches an equality. In the case of condensation, the signs in the inequalities are reversed.

The basis for subroutine WCNDNS, which computes the evaporation/condensation rate on a heat sink surface, is described here. An iterative solution finds the mass fraction of steam at the Langmuir interface (which is directly related to $P_{st,I}$) needed to equate the mass transfer rate in the Langmuir layer to that in the mass diffusion layer. This subroutine also anticipates the change in heat sink surface temperature, and the change in saturation pressure, $P_{sat}(T_w)$, due to heat sources and the latent of condensation/evaporation, h_{fg} . Key inputs to this subroutine are as follows:

- P - Bulk or free steam total pressure,
- T_w - Surface temperature,
- Mc_w - Heat capacity of the heat sink surface slab,
- Y_∞ - Mass fraction of steam in the free steam,
- Q_{in} - Other heat sources; e.g., decay heat, and
- Δt - Time step.

In the Langmuir layer, the condensation rate is given by:

$$w_{cd} = A \frac{(P_{st,I} - P_{sat}(T_w^{new}))}{\sqrt{2\pi R_v T_w^{old}}} \quad (3-49)$$

where A is the heat sink surface area, R_v is the gas constant, and the anticipated, or new, wall temperature is given by:

$$T_w^{new} = T_w^{old} + \frac{(Q_{in} + w_{cd} h_{fg}) \Delta t}{M c_w} \quad (3-50)$$

Using the Clausis-Clapeyron equation, estimate the saturation pressure at the new wall temperature by:

$$P_{sat}(T_w^{new}) = P_{sat}(T_w^{old}) + (T_w^{new} - T_w^{old}) \frac{h_{fg}}{T_w^{old} v_{fg}} \quad (3-51)$$

Substituting equation (3-50) into equation (3-51),

$$P_{sat}(T_w^{new}) = P_{sat}(T_w^{old}) + \frac{(Q_{in} + w_{cd} h_{fg}) \Delta t}{M c_w} \frac{h_{fg}}{T_w^{old} v_{fg}} \quad (3-52)$$

Substitute equation (3-52) into equation (3-49) and factor out w_{cd} to obtain:

$$w_{cd} = A \frac{\left(P_{st,I} - P_{sat}(T_w^{old}) - \frac{Q_{in} h_{fg} \Delta t}{M c_w T_w^{old} v_{fg}} \right)}{\sqrt{2\pi R_v T_w^{old}} \left(1 + \frac{A \frac{h_{fg}}{T_w^{old} v_{fg}} h_{fg} \Delta t}{\sqrt{2\pi R_v T_w^{old}} M c_w} \right)} \quad (3-53)$$

Now, the partial pressure of steam at the interface is given by:

$$P_{st,I} = P \frac{Y_I MW_{nc}}{Y_I MW_{nc} + (1 - Y_I) MW_{st}} \quad (3-54)$$

where Y_I is the mass fraction of steam at the outer interface of the Langmuir layer and MW is the molecular weight, with subscripts for non-condensibles and steam.

Rearrange equation (3-54):

$$P_{st,I} = P \frac{MW_{nc}}{(MW_{nc} - MW_{st})} \frac{Y_I}{Y_I + \frac{MW_{st}}{(MW_{nc} - MW_{st})}} \quad (3-55)$$

Substituting equation (3-55) into equation (3-53) gives,

$$w_{od} = C_1 \left(\frac{Y_I}{Y_I + C_2} \right) + C_3 \quad (3-56)$$

$$\text{where } C_1 = A \frac{P \frac{MW_{nc}}{(MW_{nc} - MW_{st})}}{\sqrt{2\pi R_v T_w^{old}} \left(1 + \frac{A \frac{h_{fg}}{T_w^{old} v_{fg}}}{\sqrt{2\pi R_v T_w^{old}}} \frac{h_{fg} \Delta t}{M c_w} \right)}, \quad (3-56a)$$

$$C_2 = \frac{MW_{st}}{(MW_{nc} - MW_{st})}, \text{ and} \quad (3-56b)$$

$$C_3 = \frac{-A \left(P_{sat}(T_w^{old}) + \frac{Q_{in} h_{fg} \Delta t}{M c_w T_w^{old} v_{fg}} \right)}{\sqrt{2\pi R_v T_w^{old}} \left(1 + \frac{A \frac{h_{fg}}{T_w^{old} v_{fg}}}{\sqrt{2\pi R_v T_w^{old}}} \frac{h_{fg} \Delta t}{M c_w} \right)} \quad (3-56c)$$

In the mass diffusion layer, the mass transfer rate is controlled by the diffusion equation:

$$w_{od} = C_4 \ell n (1 - Y_I) + C_5 \quad (3-57)$$

$$\text{where } C_4 = A \frac{h_c}{c_{pg}} \left(\frac{Pr}{Sc} \right)^{0.66}, \text{ and} \quad (3-57a)$$

$$C_5 = -A \frac{h_c}{c_{pg}} \left(\frac{Pr}{Sc} \right)^{0.66} \ell n (1 - Y_\infty) \quad (3-57b)$$

The constant C_4 stems from the Chilton-Colburn analogies, where h_c is the convective heat transfer coefficient, c_{pg} is the free steam gas specific heat, and Pr and Sc are the Prandtl and Schmidt numbers, respectively.

The subroutine WCNDNS iterates for the mass fraction of steam in the interface between the Langmuir layer and the diffusion layer which matches the mass transfer rates (w_{cd}) in the two layers. That is, WCNDNS solves for the root of the non-linear equation,

$$f(Y_I) = C_1 \left(\frac{Y_I}{Y_I + C_2} \right) + C_3 - C_4 \ell n (1 - Y_I) - C_5 \quad (3-58)$$

which has the derivative given by

$$f'(Y_I) = \frac{C_1 C_2}{(Y_I + C_2)^2} + \frac{C_4}{(1 - Y_I)} \quad (3-59)$$

A combination of Newton-Raphson and bisection methods is used to find the root bracketed between 0.99999 and $\text{Min}(0.9999, Y_\infty)$. If the function evaluated at $Y_I = 0.99999$ is negative, i.e., the root of the function lies outside the upper bound, then the mass transfer rate is considered to be controlled by the Langmuir equation only and the mass transfer rate given by equation (3-56) at $Y_I = 1.0$ is returned. This condition normally occurs during boiling. Otherwise, the root is refined until its accuracy is known within $\pm 10^{-5}$.

3.8.1 Implicit Method for Steam Partial Pressure

The partial pressure of the steam P_{st} changes with evaporation/condensation. Therefore, an implicit scheme is used to estimate the evaporation rate based on the end of the time-step steam partial pressure and avoid "overshooting". The partial pressure at the end of the timestep is anticipated by:

$$P_{st}^* = P_{st} + P \frac{\frac{dM_{st}}{dt} \Delta t - \sum_{i=1}^n W_{ci} \Delta t}{M_w N_g} \quad (3-60)$$

where P_{st} = steam partial pressure,
 P_{st}^* = anticipated steam partial pressure,
 P = total pressure,
 $\frac{dM_{st}}{dt}$ = rate-of-change in steam mass due to other processes,
 Δt = timestep,
 W_{ci} = condensation rate, and
 N_g = total gas moles.

The index "i" refers to the heat sink surfaces in the region. The condensation rate is linearized as follows:

$$W_{ci} = \left. \frac{dW_c}{dP_{st}} \right|_i (P_{st}^* - P_{sat}(T_i^*)) \quad (3-61)$$

where T_i^* is the temperature of heat sink "i" after other heat sources, such as decay heat, oxidation heat, and latent heat are considered, and the rate-of-change of condensation with respect to partial pressure is approximated as:

$$\left. \frac{dW_c}{dP_{st}} \right|_i = \frac{W_{ci}^o}{P_{st} - P_{sat}(T_i^*)} \quad (3-62)$$

where W_{ci}^o is the condensation rate determined in the previous section.

Substituting equation (3-61) into equation (3-60),

$$P_{st}^* = P_{st} + \frac{P}{M_w N_g} \left(\frac{dM_{st}}{dt} \Delta t - \sum_i \frac{dW_c}{dP_{st}} \bigg|_i (P_{st}^* - P_{st} \langle T_i^* \rangle) \Delta t \right) \quad (3-63)$$

Or, after rearranging,

$$P_{st}^* = \frac{P_{st} + \frac{P \Delta t}{M_w N_g} \left(\frac{dM_{st}}{dt} + \sum_i \frac{dW_c}{dP_{st}} \bigg|_i P_{sat} \langle T_i^* \rangle \right)}{1 + \frac{P \Delta t}{M_w N_g} \sum_i \frac{dW_c}{dP_{st}} \bigg|_i} \quad (3-64)$$

Once the anticipated partial pressure of steam in the region is determined, equation (3-61) can be evaluated for each surface for the condensation rate.

3.8.2 Implementation in the Code

Evaporation and condensation of water on individual fuel/scrap heat sink is calculated in subroutine EVPCND. Actually, subroutine EVPCND is called twice for each heat sink. During the first pass, each individual heat sink surface is visited. Subroutine EVPCND calls function routine WCNDNS to determine the mass transfer rate and estimate the $\frac{dW_c}{dP_{st}} \bigg|_i$ term. The first pass is repeated up to six times until the bulk steam partial pressure is converged.

Then, during the second pass, the actual condensation/evaporation rates are computed based on the end-of-time step bulk steam partial pressure. Also, appropriate rate terms are updated to reflect mass and energy transfer during the condensation/evaporation. For fuel rods, the latent heat is added to the surface. For scrap basket, the heat is distributed volumetrically. Figures (3-12), (3-13), and (3-14) show the calculation steps.

3.9 Radiolysis

Radiolytic gas generation can be divided into two parts: (1) gas generation due to sludge water, and (2) gas generation due to free water. The sludge water part of the model is based on the empirical relationship from [Pajunen, 1997]. Inputs to the empirical relationship are the

Figure 3-12: Flowchart for Evaporation/Condensation Rate Calculation.

Figure 3-13: Flowchart for Subroutine EVPCND (IMODE = 0).

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Figure 3-14: Flowchart for Subroutine EVPCND (IMODE = 1).

SL984111.CDR 4-24-98

fractional heat loads from alpha, beta, and gamma radiation. Output is expressed in G values, which are the number of molecules of gas (H_2 or O_2) generated per 100 ev absorbed by particulate matrix. G values are summarized as follows:

Table 3-5: Radiolytic Gas Generation in a Drained/Dried Multi-Canister Overpack (Units in molecules/100 ev absorbed by particulate matrix)		
Radiation Type	G_{H_2}	G_{O_2}
Alpha	$1.5(x_w)$	$0.75(x_w)$
Beta	$0.45(x_w)$	$0.225(x_w)$
Gamma	$30(x_w)$ for $0 \leq x_w \leq 0.04$ 1.2 for $0.04 < x_w \leq 0.35$ $1.604-1.154(x_w)$ for $0.35 < x_w \leq 1$	$1(x_w)$ for $0 \leq x_w \leq 0.225$ 0.225 for $0.225 < x_w \leq 1$
Notes: 1) x_w = mass fraction water in the fuel particulate. 2) The G values for beta radiation are based on the linear energy transfer from beta energies approximating ^{90}Sr , ^{90}Y , and ^{137}Ca decay, which dominate beta radiation from N reactor fuel. Higher G values from beta radiation would be predicted if lower energy beta radiation (e.g., 3H decay) dominates the energy source.		

For free water, G values are 0.45 for hydrogen and 0.225 for oxygen. The other major input for the free water radiolysis model is Q - the photon heat deposition rate in MCO free water per gram per MTU of fuel loading. Lan found an average heat deposition rate in MCO free water of 1.17×10^{-5} W/gm; peak values were 30% higher [Lan, 1996].

3.10 Nitriding

HANSF nitriding models are based on the rate laws of Mallett and Gerds. Fuel nitriding is expressed by:

The nitriding model uses the same fuel basket and scrap basket reaction areas as the oxidation model, although a nitriding multiplier is provided to account for uncertainties in reaction area, rate laws, etc. HANSF deposits the nitriding heat of reaction in the fuel element surface, but deposits the nitriding heat of reaction throughout the entire scrap basket heat sink volume.

Rate laws are modeled as follows. For temperatures less than 750°C,

$$k = 202 \exp \left(\frac{-25,500}{RT} \right) \quad (\text{ml/cm}^2)^2/\text{s} \quad (3-71a)$$

and for temperatures in the range between 775 and 900°C,

$$k = 3.95 \exp \left(\frac{-15,500}{RT} \right) \quad (\text{ml/cm}^2)^2/\text{s} \quad (3-71b)$$

where T is degrees in K, and R is the gas constant (cal/mole-K). HANSF linearly interpolates to find k for temperatures between 750 and 775°C. Rate constant k is converted to units of (kg/m²)²/s by multiplying by the square of the density of nitrogen at STP and a conversion factor.

4.0 CODE ARCHITECTURE

4.1 Main Program Organization

The main HANSF routine is a driver that performs the following tasks:

- (1) Gathers input and initializes region routines,
- (2) Calls routines to determine auxiliary variables (pressure and temperature) and thermophysical properties based on pressure and temperature,
- (3) Calls routines for timestep control and statistics,
- (4) Calls routines to calculate the rates-of-change of state variables (mass and energy) in each region,
- (5) Calls routines to integrate state variable quantities, and
- (6) Calls routines to create HANSF output.

A flowchart of the main HANSF routine is shown in Figure 4-1. The flowchart is explained below.

GETFIL processes the input file name and GASPROP.DAT,

HSINI initializes heat temperatures and properties,

BNDSET imposes fixed boundary conditions to designated region pressures and heat sinks. BNDSET is called once as part of the code initialization, and is then called at the beginning of each timestep to impose user-defined boundary conditions,

REGINI initializes the region for mass and energy. Region initial conditions are expressed in terms of pressure, temperature, and gas mole fractions. REGINI computes region mass and energy based on these inputs for initial conditions, PLTIN prepares plot variables and the plot file header. HANSF creates a file with a PLT extension that contains output values for plotting. Section 6.2

Figure 4-1: HANSF Main Program Flowchart.

describes the plot file. The user specifies the plot variables from a list of possible choices,

RESTRT handles the code restart capability. This capability saves run time and facilitates parametric runs. Suppose a user wants to vary a boundary condition at 15,000 seconds and perform several parametric runs. The user makes an initial run that lasts a little more than 15,000 seconds. Then the user can perform several restarts from the first run, with a different boundary condition each time. This saves the expense of needlessly running out to 15,000 seconds each time. RESTRT necessarily operates in two modes: the first mode is to read a restart file that is used for the current run, the second mode is to write a restart file that can be used in a later run. In the flowchart, these are denoted by RESTRT(0) and RESTRT(1), respectively. When RESTRT is called in Mode 0, the code reads an existing file (with an RER extension) for the values of state variables, extrapolated pressure and temperature, and junction flowrates, both unidirectional and counter-current,

TIMCON determines time-dependent time step, restart interval, output interval, and plot frequency,

PTREG calculates temperature and pressure for each region based on mass and energy. The basis for this subroutine is given in the discussion on region thermodynamics (Section 3.0),

PROPO determines gas mixture properties based on temperatures and pressures from PTREG,

HSAVG computes heat sink average temperature,

TDSET is called to determine the limiting timestep before rates are calculated,

RATES computes the rates-of-change of the region state variables,

TDSET is called after rates have been calculated to provide timestep statistics,

OUTPUT writes to the tabular output file,

PLTOUT writes to the main plot file,

PLTOUTMCO writes to the MCO plot file, and

INGRAT performs the first-order Euler integration.

4.2 Subroutine and Function Descriptions

HANSF subroutine and function names are listed below, along with a brief description of each:

AERDIS	-	Aerosol size distribution function.
AEROSL	-	Aerosol settling and leakage for all regions.
AXCOND	-	Subroutine for axial conduction and conduction networks.
BASFLO	-	Scrap basket flow split.
BNDSET	-	Sets user-defined boundary conditions.
CONIN	-	Read CONTROL section input.
COPYFL	-	Duplicates input for an MCO fuel basket.
COPYHS	-	Duplicates input for a heat sink.
COPYSC	-	Duplicates input for a scrap basket.
CORROD	-	Oxidation of fuel in either the fuel basket or the scrap basket.
DEENTR	-	Particle de-entrainment due to 90 degree bends.
DEHYDR	-	Dehydration of uranium hydrates in sludge.
DIX	-	Mixture diffusion coefficient using Blanc's law.
DSOLV1	-	Mathematical utility for solving a system of linear equations; decompose a matrix into lower and upper triangular matrices.
DSOLV2	-	Mathematical utility for solving a system of linear equations.
EVPCND	-	Evaporation/condensation of water vapor on heat sink surfaces.
FCOND	-	Condensation rates.
FOG	-	Fog formation/evaporation for all regions.
FPSAT	-	Fit to Keenan and Keyes water vapor saturation curve.

GASINP	-	Read in gas property data.
GAST	-	Gas mass and mole fractions, total mass and moles, formula weight.
GETCLI	-	Gets and returns the command line string following the executable name.
GETGAS	-	Read gas or aerosol inputs.
GETFIL	-	Gets input file name.
GRAYNC	-	Multi-body radiation between grey heat sinks.
HANSIN	-	Main input routine.
HGSRG	-	Applies a gas source to state variable rate terms.
HMICCV	-	Micro-convection heat transfer in a narrow enclosure.
HSAVG	-	Computes average heat sink temperature.
HSIN	-	Heat sink input and initialization.
HSREG	-	Heat sink temperature distribution.
HTCND	-	Solution scheme for condensate film interface temperature.
HYDRID	-	Creation and conversion of hydride particles on uranium fuel.
ICGET	-	Space-saving routine for junction inputs.
IGNAM	-	Get gas index given its name.
INGRAT	-	Performs the first-order Euler integration for state variables.
INSERT	-	Inserts a heat sink into a conduction network.
INTNUM	-	Returns integer number of a character word.
IRCGET	-	Space-saving routine for junction inputs.
ISCGET	-	Space-saving routine for column style inputs.
ISCHAR	-	Returns the ASCII definition a character if it is a valid character, and makes the character uppercase if necessary.

ISNUM1	-	Function to return a positive value of digit number if character is a number, else returns -1.
JFLOW	-	Computes inter-compartmental gas flows through junctions.
JUNCIN	-	Junctions input.
KGMIX	-	Calculates gas thermal conductivity.
LAMSED	-	Aerosol settling removal constant.
LENF	-	Finds number of characters in a string.
LOOK2	-	Linear interpolation routine.
LOOKTM	-	Determines plot output, plot, and minimum and maximum time steps based on user-input.
LOOKUP	-	Linear interpolation routine.
LTERP	-	Locates interpolation arrays.
MCO	-	Subroutine for MCO phenomena: (1) radiative heat transfer between fuel nodes, (2) conduction heat transfer between the fuel nodes, (3) decay heat source, (4) oxidation of fuel, (5) hydriding, (6) evaporation and condensation of water on a fuel element and structure surfaces, (7) solar radiation, (8) hydrate decomposition, (9) radiolysis, and (10) nitriding.
MCOIN	-	MCO input routine.
MISPEL	-	Checks misspelled words in input file.
MUM	-	Gas mixture viscosity using Brokaw approximation.
NCOROD	-	Nitriding of fuel in either the scrap basket or fuel assembly.
OUTPUT	-	Prints tabular output.
PACK	-	Removes blanks between the label and the integer index in a character string.
PLSET1	-	Sets logical flag for plotting of variables stored as a vector.
PLSET2	-	Sets logical flag for plotting of variables stored as an array.

PLTIN	-	Reads plot variables and sets up main plot file header.
PLTINMCO	-	Reads plot variables and sets up MCO plot file header.
PLTOUT	-	Controls main plot output.
PLTOUTMCO	-	Writes MCO plot output.
PR TIN	-	Reads print variables and checks for misspellings.
PRTMCO	-	Calculates MCO output.
PROP0	-	Calculates mixture properties of gases.
PTREG	-	Driver for multi-region pressure and temperature with non-ideal gases. Calls PTREG1.
PTREG1	-	Pressure and temperature with non-ideal gases in a single region.
PTREGE	-	Equilibrium of vapors and condensed fogs.
RADIOL	-	Computes radiolytic gas generation rates.
RATES	-	Assembles the rates-of-change for all state variables.
RDARI	-	Reads in the array input parameter and echoes back the data.
RDARR	-	Reads in the array input parameter and echoes back the data.
RDARR1	-	Reads in two real array inputs and echoes back the data.
RDMTI	-	Reads in the matrix of numbers.
RDMTR	-	Reads in the array input parameter and echoes back the data.
REGINI	-	Initializes a single region for mass and energy, given pressure and temperature.
REGINJ	-	Reads VOLUMES input.
REGVAL	-	Initialize set of regions with non-ideal gases.
RELNUM	-	Returns a real number of a character word.
RESTR T	-	Handles restart read and write.

RTGPX	-	Provides rates-of-change of gas pressure and temperature; used only when there are no junctions.
RXHYD	-	Block & Mintz hydriding/dehydriding rate law.
SCRIMP	-	Impaction in the scrap basket.
SENSE	-	Handle sensitivity runs (developmental).
SORTBK	-	Sorts the baskets according to position.
SOURCE	-	Rates-of-change due to user-specified sources of mass and energy.
STAMPINL	-	Gets directory path and file data of input file for Lahey compiler.
STAMPINM	-	Gets directory path and file data of input file for Digital Visual Fortran compiler.
STRCOP	-	Concatenates strings.
TDSET	-	Provides timestep selection and statistics.
TIMCON	-	Determines max/min time step, restart interval, output interval, and max/min plot frequency.
TOKEN	-	Parses tokens from a line delimited by space or comma.
TOKENL	-	Reads a line and calls TOKEN.
TRIDAG	-	Tri-diagonal matrix solver: $A_n X_{n-1} + B_n X_n + C_n X_{n+1} = D_n$
TSOFP	-	Inverse of saturation pressure correlations.
WCNDNS	-	Condensation, evaporation and boiling on a heat sink surface.
WJEX0	-	Initializes counter-current flow routine.
WJEXCH	-	Calculates counter-current flow through junctions; calculates flooding flowrate.
WRXUN	-	Provides uranium metal (or hydride) nitriding rate.
WRXUO	-	Provides uranium metal (or hydride) oxidation reaction rate.

4.3 Subroutine and Function Calls

The listing below describes the subroutine and function calls that HANSF makes:

HANSF : Main Program
 Calls: GETFIL, BNDSET, SENSE, REGINI, PLTIN, RESTRT, PTREG,
 PROPO, HSAVG, TDSET, RATES, OUTPUT, PLTOUT, INGRAT,
 PLTOUTMCO, TIMCON

AMDAT : Block Data

AERDIS : Subroutine
 Calls: LTERP
 Called by: FOG

AEROSL : Subroutine
 Calls: DEENTR, LAMSED
 Called by: RATES

AXCOND: Subroutine
 Calls: TRIDAG
 Called by: HSREG, MCO

BASFLO : Subroutine
 Called by: MCO

BNDSET : Subroutine
 Calls: LOOK2
 Called by: HANSF

CONIN : Subroutine
 Calls: PLTIN, TOKENL, RELNUM, INTNUM, IGNAM, MISPEL, PRTIN,
 RDARR, RDARR1
 Called by: HANSIN

COPYFL, COPYSC, COPYHS : Subroutines
 Called by: MCOIN

CORROD : Subroutine
 Calls: WRXUO, HGSRC
 Called by: MCO

DEENTR : Subroutine
Calls: LTERP, MUM
Called by: AEROSL

DEHYDR : Subroutine
Calls: IGNAM, WCNDNS
Called by: MCO

DSOLV1 : Subroutine
Called by: JFLOW, GRAYNC

DSOLV2 : Subroutine
Called by: JFLOW, GRAYNC

EVPCND : Subroutine
Calls: WCNDNS, IGNAM
Called by: MCO

FOG : Subroutine
Calls: PTREGE, AERDIS
Called by: RATES

GASINP : Subroutine
Calls: TOKENL, RELNUM, MISPEL
Called by: GETFIL

GAST : Subroutine
Calls: None
Called by: PTREG, JFLOW

GETCL1 : Subroutine
Calls: NARGS, GETARG, STRCOP, LENF, LEN
Called by: GETFIL

GETFIL : Subroutine
Calls: GETCL1, TOKENL, LENF, HANSIN, GASINP
Called by: HANSF

GETGAS : Subroutine
Calls: INTNUM, TOKENL, IGNAM, RELNUM
Called by: REGINJ

GRAYNC : Subroutine
Calls: DSOLV1, DSOLV2
Called by: MCO, HSREG

HANSIN : Subroutine
 Calls: TOKENL, CONIN, INTNUM, REGINJ, HSIN, JUNCIN, MCOIN, MISPEL
 Called by: GETFIL

HSAVG : Subroutine
 Calls: IGNAM, LOOKUP
 Called by: HANSF

HSIN : Subroutine
 Calls: TOKENL, INTNUM, ICGET, IRCGET, RELNUM, RDARR, RDARR1, RDMTR, MISPEL
 Called by: HANSIN

HSREG : Subroutine
 Calls: HTCND, TRIDAG, AXCOND, GRAYNC
 Called by: RATES

HTCND : Subroutine
 Calls: FCOND
 Called by: HSREG

HYDRID : Subroutine
 Calls: RXHYD, HGSRC
 Called by: MCO

INGRAT : Subroutine
 Called by: HANSF

INSERT : Subroutine
 Called by: MCOIN

JFLOW : Subroutine
 Calls: WJEX0, WJEXCH, PTREG1, DSOLV1, DSOLV2, GAST
 Called by: RATES

JUNCIN : Subroutine
 Calls: TOKENL, INTNUM, ICGET, IRCGET, MISPEL
 Called by: HANSIN

LOOKTM : Subroutine
 Called by: TIMCON

LTERP : Subroutine
 Called by: AERDIS, DEENTR, SCRIMP

MCO : Subroutine
Calls: AXCOND, IGNAM, PRTMCO, GRAYNC, HMICCV, CORROD,
HYDRID, EVPCND, LOOK2, BASFLO, SCRIMP, DEHYDR, HGSRC,
NCOROD, RADIOL, SCRIMP, SORTBK
Called by: RATES

MCOIN : Subroutine
Calls: TOKENL, INTNUM, RELNUM, RDARR, RDARI, RDMTR, RDMTI,
COPYFL, COPYHS, COPYSC, INSERT, PLTINMCO
Called by: HANSIN

NCOROD : Subroutine
Calls: WRXUN
Called by: MCO

OUTPUT : Subroutine
Calls: PRTMCO
Called by: HANSF

PACK : Subroutine
Called by: PLTINMCO

PLSET1 : Subroutine
Calls: INTNUM
Called by: PLTIN, PRTIN

PLSET2 : Subroutine
Calls: IGNAM, INTNUM
Called by: PLTIN

PLTIN : Subroutine
Calls: LENF, MISPEL, PLSET1, PLSET2, TOKENL
Called by: CONIN, HANSF

PLTINMCO: Subroutine
Calls: LENF, PACK
Called by: MCOIN

PLTOUT : Subroutine
Called by: HANSF

PLTOUTMCO: Subroutine
Calls: IGNAM
Called by: HANSF

PROPO : Subroutine
Calls: MUM, IGNAM, DIX, KGMIX
Called by: HANSF

PRTIN : Subroutine
Calls: MISPEL, PLSET1, TOKENL
Called by: CONIN

PRTMCO : Subroutine
Called by: MCO, OUTPUT

PTREG : Subroutine
Calls: PTREG1, GAST, PTREG2
Called by: HANSF

PTREG1 : Subroutine
Called by: PTREG, JFLOW, PTREG2

PTREGE : Subroutine
Called by: FOG

RADIOL : Subroutine
Called by: MCO

RATES : Subroutine
Calls: MCO, SOURCE, HSREG, FOG, JFLOW, RTGPX, AEROSL
Called by: HANSF

RDARI : Subroutine
Calls: TOKENL, INTNUM
Called by: MCOIN, HSIN

RDARR : Subroutine
Calls: TOKENL, RELNUM
Called by: REGINJ, HSIN, MCOIN, CONIN

RDARR1 : Subroutine
Calls: TOKENL, RELNUM
Called by: CONIN

RDMTI : Subroutine
Calls: TOKENL, INTNUM
Called by: MCOIN

RDMTR : Subroutine
Calls: TOKENL, RELNUM
Called by: MCOIN, HSIN

REGINI : Subroutine
Calls: REGVAL
Called by: HANSF

REGINJ : Subroutine
Calls: TOKENL, INTNUM, IRCGET, GETGAS, RDARR, RELNUM, MISPEL
Called by: HANSIN

REGVAL : Subroutine
Called by: REGINI

RESTRT : Subroutine
Called by: HANSF

RTGPX : Subroutine
Called by: RATES

SCRIMP : Subroutine
Calls: LTERP, MUM
Called by: MCO

SENSE : Subroutine (not functioning)
Called by: HANSF

SORTBK : Subroutine
Called by: MCO

SOURCE : Subroutine
Calls: HGSRC
Called by: RATES

STAMPINL: Subroutine
Calls: LENF, TOKENL
Called by: GETFIL

STRCOP : Subroutine
Calls: LENF
Called by: GETCL1

TDSET : Subroutine
Called by: HANSF

TIMCON : Subroutine
 Calls: LOOKTM
 Called by: HANSF

TOKEN : Subroutine
 Calls: ISCHAR, LEN
 Called by: TOKENL

TRIDAG : Subroutine
 Called by: HSREG, AXCOND

WJEX0 : Subroutine
 Called by: JFLOW

WJEXCH : Subroutine
 Called by: JFLOW

DIX : Function
 Called by: PROP0

FCOND : Function
 Calls: IGNAM, WCNDNS
 Called by: HTCND

FPSAT : Function
 Called by: WRXUO

HGSRC : Function
 Called by: SOURCE, MCO, HYDRID, CORROD

HMICCV : Function
 Called by: MCO

ICGET : Function
 Calls: INTNUM
 Called by: HSIN, ICGET, JUNCIN

IGNAM : Function
 Called by: CONIN, GETGAS, PROP0, FCOND, MCO, TOKENL, EVPCND,
 HSAVG, PLSET2, PLTOUTMCO

INTNUM : Function
 Calls: ISNUM1, LEN
 Called by: HANSIN, CONIN, REGINJ, GETGAS, HSIN, JUNCIN, ICGET,
 RDARI, MCOIN, RDMTI, TOKENL, PLSET1, PLSET2

IRCGET : Function
 Calls: RELNUM
 Called by: REGINJ, HSIN, JUNCIN

ISCHAR : Function
 Called by: TOKEN

ISNUM1 : Function
 Called by: RELNUM, INTNUM

KGMIX : Function
 Called by: PROP0

LAMSED : Function
 Called by: AEROSL

LENF : Function
 Calls: LEN
 Called by: TOKENL, GETFIL, STRCOP, GETCL1, PLTIN, MISPEL,
 PLTINMCO, STAMPINL

LOOKUP : Function
 Called by: HSAVG, MCO

MISPEL : Function
 Called by: CONIN, GASINP, HANSIN, HSIN, JUNCIN, PLTIN, REGINJ

MUM : Function
 Called by: PROP0, SCRIMP, DEENTR

RELNUM : Function
 Calls: ISNUM1, LEN
 Called by: CONIN, GETGAS, GASINP, IRCGET, RDARR, RDMTR, MCOIN,
 REGINJ, HSIN, RDARR1

RXHYD : Function
 Called by: HYDRID

S2BV : Statement function

SBV : Statement function
 Called by: PTREGE

SCP : Statement function

SCV0 : Statement function
Called by: PROPO

SDBV : Statement function
Called by: PTREGE

SHFG : Statement function
Called by: PTREGE

SK1 : Statement function
Called by: FPU3HY

SK2 : Statement function
Called by: FWU3HY

SKF : Statement function
Called by: RXHYD

SKM : Statement function
Called by: RXHYD

SPD : Statement function
Called by: RXHYD

SPV : Statement function

SRH : Statement function
Called by: OUTPUT

SRLS : Statement function

SUG0 : Statement function

SULS : Statement function

SVG : Statement function

SVV : Statement function

TOKENL : Function
Calls: LENF, TOKEN
Called by: HANSIN, CONIN, REGINJ, GETGAS, GASINP, HSIN, JUNCIN,
RDARR, RDARI, RDMTR, GETFIL, MCOIN, PLTIN, PRTIN, RDARR1,
RDMT1, STAMPINL

TSOFP : Function

WCNDNS : Function
Called by: EVPCND

WRXUN : Function
Called by: NCOROD

WRXUO : Function
Calls: FPSAT
Called by: CORROD

5.0 INPUT DESCRIPTION

Code input consists of two files: (1) a gas properties file, which contains the thermophysical properties for the species that the code will track, and (2) an input file, which contains input for control, plotting, regions, heat sinks, junctions, and MCO models. This section describes the structure and syntax of both files.

5.1 Species Properties

The structure of the gas properties file (GASPROP.DAT) is "keyword" based. That is, the code reads the first word of each line, followed by a series of numbers that define properties for the particular species. Ten lines are required to specify the properties of a species. Up to sixteen species are allowed. An example of a gas property set for nitrogen is shown in Figure 5-1. The first line must have the following format:

GAS NITROGEN	Formula Weight	Heat of Formation (J/kg)
--------------	----------------	--------------------------

Other lines in the property set can come in any order. Each line has the format of a keyword followed by a series of numbers that specify the property or value denoted by the keyword. Each is discussed below individually:

CVG is the keyword for the ideal gas constant-volume heat capacity (J/kg/K). The second "word" in this line is a test temperature to check the heat capacity fit. The third "word" is the known ideal gas heat capacity value at the test temperature. HANSF computes C_v based on the specified fit and test value, and compares the computed value with the known one. Words four through eight correspond to A through E for the following fit:

$$CVG = A + BT + CT^2 + DT^3 + ET^4 \quad (5-1)$$

An error message is produced if the line does not contain eight words.

Figure 5-1: Gas Properties Set for Nitrogen.

GAS NITROGEN	2.80130E+01	0.00000E+00			
CVG 1.50000E+03	947.	7.42319E+02	-1.38235E-01	4.78640E-04	4.14112E-11
BV 1.40000E+03	0.0001286	1.66786E-03	-5.33929E-01	-2.18321E+03	-1.65357E+14
FV 126.100E+00	3.3818E6	5.9826E1	-1.0976E3	-8.6689E0	1.0E0
HFG 300.	0.E0	0.E0	0.E0	0.E0	0.E0
KG 0.026	0.0323	0.0393	0.044	6.775E1	0.E0
MUG 1.5E3	5.3917E-5	7.632E-7	5.8823E-1		
DFG 3.798	71.4	0.E0	1.E0	1.E0	0.E0
RL 300.	1.E-3	1.E-3	0.E0	0.E0	0.E0
CVL 300.	1.E3	1.E3			

CVL is the keyword for the liquid heat capacity (J/kg/K). The line for CVL has the same format as that for CVG.

BV is the keyword for the second virial coefficient (m^3/kg). The second word is the temperature to test the fit, and the third is the check value. Words four through eight correspond to A through E in the following fit:

$$BV = A + B/T + C/T^3 + D/T^8 + E/T^9 \quad (5-2)$$

PV is the keyword for vapor pressure (Pa), followed by a critical temperature, pressure at the critical temperature, and coefficients A through E for the following fit:

$$PV = \text{EXP} (A + B/T + C \log(T) + DT^E) \quad (5-3)$$

HFG is the keyword for heat of vaporization (J/kg), followed by a test temperature, the value at the test temperature, and the coefficients to the following fit:

$$\text{HFG} = A (1 - T_R)^{(B + CT_R + DT_R^2 + ET_R^3)} \quad (5-4)$$

where T_R is the reduced temperature.

RL is the keyword for density (kg/m^3), followed by a test temperature, a value at the test temperature, and coefficients for the following fit:

$$RL = A + BT \quad (5-5)$$

MUG is the keyword for vapor dynamic viscosity ($\text{N}\cdot\text{s}/\text{m}^2$), followed by a test temperature, the value at that temperature, and coefficients for the following fit:

$$\text{MUG} = \frac{AT^B}{1 + C/T + D/T^2} \quad (5-6)$$

KG is the keyword for gas thermal conductivity ($\text{W}/\text{m}\cdot\text{K}$), followed by four coefficients. The coefficients are used in the following formulas:

$$KG = A + (B - A) \left(\frac{T - 300}{100} \right) \quad \text{if } T < 400 \text{ K} \quad (5-7)$$

$$KG = B + (C - B) \left(\frac{T - 400}{100} \right) \quad \text{if } 400 \text{ K} < T < 500 \text{ K} \quad (5-8)$$

$$KG = C + (D - C) \left(\frac{T - 500}{100} \right) \quad \text{if } T > 500 \text{ K} \quad (5-9)$$

DFG is the keyword for diffusion coefficient, followed by SIG, EK, and DEL, which are the Lennard-Jones and Stockmayer potential parameters [Reid, et al.,

1977]. Units for SIG and EK are angstroms and degrees Kelvin, respectively; DEL is dimensionless.

5.2 Input File

The input file provides input to control execution and describe active models, sources, volumes, heat sinks, junctions, and MCO-specific input. A complete example is shown in Appendix B. Input files are fully keyword-based and broken up into the following sections: CONTROL, VOLUMES, HEAT_SINKS, JUNCTIONS, and MCO. There is a keyword for each section, which means that these sections can be arranged in any order, and the user is free to tab and indent the input file into any convenient format. Each major section has sub-sections, also designated by keywords.

The overall input file structure is:

```
CONTROL
  Sub-Section Keywords
END

VOLUMES
  Sub-Section Keywords
END

HEAT_SINKS
  Sub-Section Keywords
END

JUNCTIONS
  Sub-Section Keywords
END

MCO
  Sub-Section Keywords
END
```

Because the input file is keyword-based, these major sections can be arranged in any order. Lines whose first token is "*" are always comments. Non-keyword lines are comments by

default, but they should be used only when keywords are expected, and not when numerical values are expected. Except where noted, units in the SI (MKS) system are required. Temperature inputs are in degrees C, and pressure is in Pascals. Syntax for each major section is described below.

5.2.1 CONTROL Section

The CONTROL section provides input to designate the title and control timing, plotting, the type of active modeling, and mass and energy sources to each control volume. The syntax for this section consists of keywords for sub-sections, as follows:

CONTROL

TITLE

Any lines between these keywords are echoed as the title.

END

TIMING

List of keywords and values.

END

ACTIVE

List of keywords and values.

END

PLOT

List of keywords and values.

END

PRINT

List of keywords and values.

END

END

The syntax for each sub-section is described below.

5.2.1.1 TITLE Sub-Section

Any lines between the keywords are echoed in the output files as the title. For example, for the following TITLE sub-section,

```
TITLE
  MCO Base Case
END
```

the title "MCO Base Case" will appear in the tabular output, plot and log files that are described in Section 6.0.

5.2.1.2 TIMING Sub-Section

The TIMING sub-section contains number values for the variables to control code execution. An example of syntax is as follows:

```
TIMING
  TSTART    0.0      !START TIME
  TLAST     300      !END TIME
  DTMIN      2.      !MIN TIMESTEP
  DTMAX      5.      !MAX TIMESTEP
  DPTRIN     30.     !PRINT INTERVAL
  FTPCH      0.03    !FRACTIONAL CHANGE IN T AND P
  FAECH      0.03    !FRACTIONAL CHANGE IN AEROSOL MASS
  PLTMIN      2.0     !MINIMUM PLOT INTERVAL
  PLTMAX      5.0     !MAXIMUM PLOT INTERVAL
  FPPLCH      0.1    !FRAC RATE OF CHANGE FOR PLOT POINT
  DTRST     100.0    !RESTART INTERVAL
END
```

Since the input is keyword-based, the order of the input is irrelevant as long as the keywords are placed between the TIMING and END keywords. That is, TLAST can come before TSTART if the user desires. Of course, TLAST must be larger than TSTART; otherwise, the code stops execution after initialization.

Choices for DTMIN and DTMAX are a matter of judgement, with a few things that the user must bear in mind. First, DTMIN is the minimum time step that the code will use,

regardless of the rate-of-change limitations posed by FTPCH or FAECH. DTMAX is the maximum time step the code will use, assuming that there are no limitations brought about by the rate-of-change logic. DTMAX should generally be several multiples of DTMIN, and could be an order of magnitude higher than DTMIN in a long transient where pertinent rates-of-change will vary significantly. The fractional rate-of-change logic controls time step. At the first time step, this logic begins by assuming DTMIN as the initial time step. Thereafter, the code follows this logic:

- (1) As a trial, double the previous time step; if this exceeds DTMAX, the trial time step is set equal to DTMAX.
- (2) Compute fractional rates-of-change for region temperatures, pressures, and aerosol masses. Fractional rate-of-change, F, for some variable X, is defined as:

$$F = (dX / dt) / X \quad (5-10)$$

- (3) Compare fractional rates-of-change to limits set by FTPCH and FAECH. If these are exceeded in any region, limit the time step to:

$$DELT = FTPCH / F \text{ (or FAECH / F)} \quad (5-11)$$

- (4) The time step then is the maximum of DELT and DTMIN.

Recommended values for both FTPCH and FAECH are anywhere between 0.01 to 0.05. PLTMIN is the minimum time interval between plot points, while PLTMAX is the maximum time interval. Logically, PLTMIN must be greater than the minimum time step. Also, it is recommended that (PLTMAX - PLTMIN) be greater than (DTMAX - DTMIN). To avoid skipping over a desired plot point, the code constrains PLTMAX to be equal to DTMAX, should the user specify that DTMAX is larger than PLTMAX. FPPLCH is the fractional rate-of-change for a plot point. If the fractional rate-of-change of temperature, pressure, or aerosol mass exceeds FPPLCH in any region, the code creates a plot point. This scheme allows the code to capture output during rapid transients without necessarily using many plot points during the entire run.

DTRST designates the time interval at which the code writes a restart. This creates a restart file named HANSF.REW. Restart runs are invoked by specifying a non-zero start time for TSTART. In a restart run, the code reads the HANSF.RER file, searches for the latest saved data prior to TSTART, and initializes all state variables to the saved data. By default, HANSF uses the input file name for restart read (RER extension) and restart write files (REW extension) and just appends the appropriate extension. For example, an input file named HANSF.INP will write restart data to HANSF.REW and read restart data from HANSF.RER, by default. The user can override this convention and from the input deck, specify a restart file with any desired file name. This done in the following manner:

```
RESTART_FILE    VACUUM.RER
```

This syntax in the CONTROL section allows the code to restart from file VACUUM.RER regardless of the input file name. The user must be careful manipulating the HANSF.REW and HANSF.RER files. After an initial (non-restart) run using, say, HANSF.DAT, the user should change the HANSF.REW file name to a new file name with an RER extension. In this way, an appropriate file will be read for a subsequent restart run.

Users can make several variables time-dependent, namely, DTMIN, DTMAX, DTPRIN, PLTMAX, PLTMIN, and DTRST. This feature allows the user to capture details during rapidly evolving parts of the simulation while minimizing execution time and output file size. For these six variables, the input values consist of two columns, the first column being time and second column being DTMIN (or DTMAX, DTPRIN, PLTMIN, PLTMAX, and DTRST). Use DTMIN as an example. In the first row, the user specifies time and a minimum time step; e.g., 0.0 seconds and 0.1 seconds. In the second row, the user specifies a new time and new minimum time step: e.g., 1000.0 seconds and 10 seconds. Up to 10 rows, or changes in minimum time step, are allowed. In this manner, the user can specify small time steps during periods when rates-of-change are significant, and specify large time steps during periods when rates-of-change are small. The same goes for the print interval, plot interval, and restart interval. An example follows:

TIMING	1. Keyword	
TSTART	0.	! START TIME, >0 FOR RESTART RUN
		! RESTART FILE IS READ FROM HANSF.RER
TLAST	11.	! END TIME (Seconds)
DTMIN		! MIN TIMESTEP KEYWORD
0.0	0.01	! USE 0.01 SEC MIN TIME STEP TO THE END
DTMAX		! MAX TIMESTEP KEYWORD
0.0	0.2	! USE 0.2 SEC MAX TIME STEP FOR FIRST 100 SEC.
100.	2.0	! THEN INCREASE THE MAX TIME STEP TO 2 SEC.
DTPRIN		! PRINT INTERVAL KEYWORD
0.0	5.	! PRINT EVERY 5 SEC. FOR FIRST 50 SEC.
50.	7200.	! THEN EVERY 7200 SEC AFTERWARD
7200.	7200.	!
PLTMIN		! MIN PLOT INTERVAL KEYWORD
0.0	0.01	! 0.01 SEC MIN PLOT INTERVAL FOR 1ST 100 SEC.
100.	100.	! INCREASE THE MIN INTERVAL TO EVERY 100 SEC.
PLTMAX		! MAX INTERVAL WITHOUT PLOT KEYWORD
0.0	1.0	! 1.0 SEC MAX PLOT INTERVAL FOR FIRST 100 SEC.
100.	1000.	! INCREASE THE MAX INTERVAL TO EVERY 1000 SEC.
DTRST		! RESTART INTERVAL KEYWORD
0.0	14400.	! RESTART EVERY 14400 SEC
FTPCH	0.005	! FRACTIONAL CHANGE IN T AND P
FAECH	0.005	! FRACTIONAL CHANGE IN AEROSOL MASS
FPFLCH	0.03	! FRACTIONAL CHANGE FOR PLOTTING

END TIMING ! TIMING is a comment.

5.2.1.3 ACTIVE Sub-Section

The ACTIVE sub-section denotes which phenomenological models will be used for a run. This sub-section has been developed primarily for code development purposes; it allows validation of individual models. The user can turn individual models on or off to save execution time (by skipping undesired subroutines) or to test for separate effects. For example, the user may wish to know if aerosol sedimentation or leakage is principally responsible for airborne aerosol removal from a particular volume. By making two runs, one with sedimentation and one without, the user can see the separate effects. One of the model parameters is a set of multipliers for effective thermal conductivities of gas in each region.

Syntax for this sub-section is as follows:

ACTIVE MODELS		! 1 = USE, 0 = DON'T USE
IJUNC	0	! INTERCOMPARTMENTAL FLOW
IHSINK	1	! HEAT SINKS
ICNDS	0	! CONDENSATION
IASED	1	! AEROSOL SEDIMENTATION
IALEAK	1	! AEROSOL LEAKAGE
IFOG	0	! FOG FORMATION
ISRC	0	! USER-DEFINED SOURCES

```

      IMCO          0          IMCO  MODELS
      ICCFLW        0          !COUNTER-CURRENT FLOW
* multipliers for region gas conductivities
* syntax:
*   FKGAS      fkgas1   fkgas2   fkgas3   ...
END

```

Only ACTIVE is necessary as a keyword, although MODELS can be added for clarity because it is interpreted as a comment. If a particular model is turned off, input for that model should be omitted or commented out. For example, if a particular runs includes no junctions (IJUNC = 0) the JUNCTIONS section should be omitted or commented out. The code will still execute with IJUNC = 0, and a correct JUNCTIONS section. If the JUNCTIONS section syntax is incorrect, however, the code will not read the input file and will not execute. The same goes for the HEAT_SINKS section if IHSINK = 0, the MCO section if IMCO = 0, etc.

5.2.1.4 SOURCES Sub-Section

The SOURCES sub-section is needed if ISRC = 1. This sub-section allows the user to specify, as a function of time, sources of gas, aerosol, and energy to a control volume. Syntax for the SOURCES sub-section is as follows:

```

C   SOURCE GROUP:  GROUPS REPEATED FOR INPUT # OF REGIONS
C   END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
C   SYNTAX EXAMPLE:
C
C   SOURCES  2
C       COMMENTS GO HERE
C   REGION 1  GASES  2
C   STEAM HYDROGEN
C       0      100.0   1.E-3   1.E-3   0.E0
C       10     100.0   1.E-3   1.E-3   0.E0
C   END
C   COMMENTS GO HERE
C   REGION 2  GASES  2
C   HYDROGEN METHANE
C       0      30.0    1.E-2   1.E-2   0.E0
C       10     30.0    1.E-2   1.E-2   0.E0
C   END
C   COMMENTS GO HERE
C   END

```

The first line consists of the SOURCES keyword, followed by the number of source groups. As shown by the example syntax, comments should be placed where keywords are expected, and

should not be placed where numbers are expected. The example above shows two source groups. The first source group is to Region 1, while the second is to Region 2. Within each source group, on the first line the first keyword is "REGION" followed by the region number, and the second keyword is "GASES" followed by the number of gases. On the second line of the source group, the gases are listed. Gas names must correspond exactly to one of the species in the GASPROP.DAT file.

Following the gas names, the source group must contain lines with numerical values for time, temperature, flowrates, and power. The number of columns in these lines must be $INGAS + 3$, where $INGAS$ is the number of gases in the source group. The columns must be in the following order: TIME, TEMPERATURE, FLOWRATES, and POWER. If there is no power to a region, the last column consists of zeros, in order to keep the number of columns at $INGAS + 3$. Up to twenty lines are allowed. The code interpolates linearly between times and at "END" creates an extra point to extrapolate. This extra point is assumed to be past the run end time (TLAST). In the first source group in the sample input above, the source of steam and hydrogen in region 1 is 1.E-3 kg/s for duration of the run.

Aerosol sources can be specified as well by using a negative region number. For example, the following input is used for the AB5 test.

SOURCES	1		
REGION	-1	GASES	1
NA2O			
0.0	300.0	4.44E-1	0.E0
10.	300.0	4.44E-1	0.E0
900.	300.0	4.44E-1	0.E0
901.	300.0	0.E0	0.E0
1.E5	300.0	0.E0	0.E0
END			
END		!END	ALL SOURCES

This input creates a sodium oxide aerosol source of 0.444 kg/s that lasts 900 seconds.

5.2.1.5 PLOTTING Sub-Section

Plot variables are specified by the following format:

```
PLOT
  Plot Variables
END
```

The following region variables can be plotted: pressure, gas temperature, heat sink temperatures, total aerosol mass (sum of all species), gas flowrate, counter-current flowrate, relative humidity, gas mass of each species, gas mole fraction of each species, total mass of each species, airborne aerosol mass of each species, and deposited liquid mass of each species. A maximum of 99 plot variables can be specified. Time and time step are always written to the plot file.

Keywords for each plot variable are as follows:

Pressure	PRESSURE
Gas Temperature	GAS-T
Heat Sink Temperature - Inner Surface	HS-TI
Heat Sink Temperature - Outer Surface	HS-TO
Heat Sink Temperature - Average	HS-TA
Aerosol Mass (Total)	AEROSOL
Mass Flowrate	GAS-W
Counter-Current Flowrate	GAS-WX
Gas Mole Fraction	GAS-X
Relative Humidity	GAS-RH
Gas Mass (Species)	GAS-MASS
Aerosol Mass (Species)	AER-MASS
Total Mass (Species)	MASS
Deposited Mass (Species)	LIQ-MASS

Two different formats are used depending on whether we are interested in a variable that needs one descriptor or a variable that needs two descriptors. Variables that need one descriptor are: pressure, temperature, heat sink temperature, total aerosol mass (all species), mass flowrate, and counter-current flowrate. Pressure, temperature, and total aerosol mass only need to have a region associated with them. Heat sink temperatures need to have an associated heat sink number. Flowrates only need a junction number. Variables that need two descriptors are: gas concentration, relative humidity, individual species gas mass, individual species aerosol mass, total (gas plus aerosol) individual species mass, and individual species deposited liquid mass. Each of these variables require a region and gas name.

For a single descriptor variable, the format is:

KEYWORD	# OF VARIABLES	REGION/HEAT_SINKS/JUNCTIONS
---------	----------------	-----------------------------

For two descriptors, the format is:

KEYWORD	GAS NAME	# OF VARIABLES	REGIONS
---------	----------	----------------	---------

An example is shown below:

PLOT			
PRESSURE	1	1	
GAS-T	2	1	2
GAS-X STEAM	2	1	2
GAS-W	1	1	
GAS-WX	1	1	
END			! END OF PLOT

This example provides plot points for the following: (1) the pressure in region 1, (2) temperatures in regions 1 and 2, (3) steam concentration in regions 1 and 2, (4) mass flowrate for junction 1, and (5) counter-current flowrate for junction 1.

5.2.1.6 PRINT Sub-Section

At the specified print interval, the following region variables are printed to an output file:

- Temperature,
- Pressure,
- Thermophysical properties,
- Gas composition in terms of mole fractions,
- Gas composition in terms of masses,
- Relative humidity of each region,
- Aerosol masses, and
- Rates-of-change of gas and aerosol.

The following variables are printed out for each junction:

- Mass flowrate, and
- Counter-current flowrate.

The following are printed out for selected heat sinks:

- Temperature degrees C of each slab, and
- Boundary conditions on each side.

The user selects which heat sinks to print out because they can be numerous for an MCO simulation. Syntax for selecting the heat sinks to be printed in the output file is as follows:

```
PRINT
  HS   3   1 2 3
END
```

In this example, output for three heat sinks, Heat Sinks 1, 2, and 3, will be printed to the output file.

5.2.2 VOLUMES Section

The next major section keyword is VOLUMES, which is followed by the number of control volumes used in the run. Up to ten control volumes are allowed. The VOLUMES major section has three sub-sections: REGIONS, AEROSOLS, and GASES. An example of the VOLUMES major section is as follows:

```
*
VOLUMES      3          ! 3 control volumes
*
  REGIONS      1          2          3
  VOLUME      0.75      0.23      1.0E9
  SED AREA    0.172     0.052     0.0
  ELEVATION    0.0       0.0       0.0
  TEMP GAS    30.00     30.00     30.00
  PRESSURE    1.013E5   1.013E5   1.013E5
END
  GASES        1          2          3
  NITROGEN    0.7775     0.7775     0.7775
  OXYGEN      0.2067     0.2067     0.2067
  STEAM       0.01579    0.0158     0.0158
  HYDROGEN    0.00001    0.00       0.00
END
END
```

Keywords REGIONS, AEROSOLS, and GASES are followed by numbers that serve as column headings for each region's data. The column headings must be in order. For each REGIONS sub-section, no more than five columns are allowed. To specify, say, seven control volumes, the user must create two REGIONS sub-sections, one with five columns of input values and one with two columns of input values. The same goes for the GASES sub-section. The GASES sub-section lists the mole fraction of each gas and should add up to 1.0 for any region. An initial aerosol loading can be specified by using the "AEROSOLS" keyword. An initial aerosol concentration is then given for each species. An example is as follows:

```
AEROSOLS      1          2          3
  NA2O        0.0001     0.0       0.0
END
```

where aerosol loading is concentration in kg/m^3 . The sedimentation area is used to determine a characteristic height for aerosol deposition; this height is simply the volume divided by the sedimentation area.

The user can impose region pressure and temperature to, say, simulate the diurnal cycle. Two real arrays specify the time-dependent conditions: the TGFIX (PGFIX) keyword is used to specify the temperature (pressure) and the TIMETG (TIMEPG) to specify the time. Clearly, the two arrays must be the same size. The code interpolates linearly between values. An example of syntax is as follows:

```

• OFFSET TIMETG
* EXTRAPOLATION TIMETG
* TIMETG REGION # TIME1, TIME2...TIMELAST
* TGFIX REGION # TEMP1, TEMP2... TEMPLAST TEMPS ARE IN C!!!
* LINEAR INTERPOLATION BETWEEN VALUES
•
* SIMILAR SYNTAX FOR PRESSURE:
* OFFSET TIMEPG
* EXTRAPOLATION TIMEPG
* TIMEPG REGION # TIME1, TIME2...
* PREFIX REGION # PRES1, PRES2...PRESSURES ARE IN PA!!!
*
* OFFSET_TIMETG= OFFSET TIME; ENTER LOOKUP TABLE WITH
*                 TIME+OFFSET_TIMETG
* EXTRAPOLATION_TIMETG= LAST TO USE LAST VALUE IN THE TABLE,
*                       = EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
*                       = PERIOD TO WRAP AROUND.
*
  OFFSET_TIMETG      50.
  EXTRAPOLATION_TIMETG LAST
  TIMETG 1 0.0 100. 200.
  TGFIX 1 30.00 30.00 30.00
*
* CONTROL MCO BOUNDARY P,
  OFFSET_TIMEPG      30.
  EXTRAPOLATION_TIMEPG EXTRAP
  TIMEPG 1 0.0 100. 200.
  PREFIX 1 1.E5 1.2E5 1.4E5

```

The "offset" feature allows the user to shift TIMETG and TIMEPG with respect to the actual simulation time. That is, $\text{TIMETG} = \text{OFFSET_TIMETG} + \text{TIME}$. In this manner, time zero can represent the start of any part of the diurnal cycle. The user specifies the diurnal cycle once, and adjusts the offset to match the time at which the simulation begins. A shipping calculation can begin at 6:00 a.m. by setting OFFSET_TIMETG to 21,600 seconds, even though the TIMETG array starts at midnight. For simulation times past the last value in TIMEPG or TIMETG, the user can choose from three options: (1) the temperature or pressure can be equal to the last value in TGFIX or PGFIX, (2) the temperature or pressure can be extrapolated from the last two points in the TGFIX or PGFIX array, or (3) the array can "wrap around" to represent periodicity. Using LAST, EXTRAP, and PERIOD, respectively, specifies these three options.

5.2.3 HEAT_SINKS Section

The HEAT_SINKS major section contains several sub-sections. One sub-section, SINKS, is always used and contains the basic inputs needed: geometry, material properties, boundary conditions, and initial conditions. The HEAT_SINKS section also contains optional sub-sections for more detailed heat sink modeling, namely material libraries, composite heat sinks, conduction networks, radiation networks, temperature-dependent emissivities, and user-defined heat sink boundary temperatures. Structure is shown below:

```

HEAT_SINKS      #      ! Major keyword and total number of heat sinks
* SINKS IS REQUIRED AND CONTAINS MOST OF THE BASIC INPUTS
  SINKS         1      2      3      4      5
  .
  .
  .
  END
  SINKS         6      7      8      9     10
  .
  .
  .
  END
.
*
* MATERIAL LIBRARY - SPECIFY MATERIAL PROPERTIES
  MATERIAL
    Name      n      (List of thermal properties)
    .
    .
    .
  END
* n is the material index for IMATHS
* SANDWICH HEAT SINKS - STRING TOGETHER NUMER OF CONSECUTIVE HEAT SINKS
  SANDWICH     (List of heat sinks and gap resistances)
.
* TEMPERATURE DEPENDENT EMISSIVITY:
  TTABLE n     (Temperature entries (C))
  ETABLE n     (Emissivity entries)
* n designates the surface
.
* CONDUCTION NETWORKS
  COND_NETWORK (Heat sink list)
.
* RADIATION NETWORKS
  RAD_NETWORK  (Heat sink list)
  FVIEW        (View factors for radiation network)
*
* USER CAN CONTROL HEAT SINK BOUNDARY TEMPERATURE
  TIMTHS IHS ISD TIME1, TIME2...
  THSFIX IHS ISD TEMP1, TEMP2...
* IHS = HEAT SINK NO.; ISD = SIDE NO. (1 OR 2)
.
END HEAT_SINKS ! HEAT_SINKS is a comment

```

Below, each of the HEAT_SINKS sub-sections is described in detail.

5.2.3.1 Basic Inputs

A simple example of syntax for the HEAT_SINKS major section is shown below:

```

HEAT_SINKS      5              ! Total of 5 sinks
*
SINKS           1             2             3             4             5
*
IGEOM           1             1             1             1             1
RHO             19100.        19100.        19100.        19100.        19100.
KHS             28.0         28.0         28.0         28.0         28.0
CPHS           116.0        116.0        116.0        116.0        116.0
QV             2000.0       2000.0       2000.0       2000.0       2000.0
XRI             0.0         0.0         0.0         0.0         0.0
XRO             0.00698     0.00783     0.00698     0.00783     0.00698
AHS             1.620       3.079       1.620       3.079       1.620
TIINIT         25.00       25.00       25.00       25.00       25.00
TOINIT         25.00       25.00       25.00       25.00       25.00
IMSLAB         3          3          3          3          3
IREGI          1          1          1          1          1
TIHS           0.0         0.0         0.0         0.0         0.0
IREGO          1          1          1          1          1
TOHS           0.0         0.0         0.0         0.0         0.0
XLHS           0.661       0.663       0.661       0.663       0.661
EHSI           0.4         0.4         0.4         0.4         0.4
EHSO           0.4         0.4         0.4         0.4         0.4
XZHS           0.661       0.663       0.661       0.663       0.661
END
*
END

```

The major keyword HEAT_SINKS is followed by the number of heat sinks. Up to 700 heat sinks are allowed. The next keyword SINKS is followed by heat sink numbers that act as column headings for heat sink inputs; the heat sink numbers must be in order. Five columns (heat sink inputs) are allowed per SINKS sub-section. To specify more than five heat sinks, repeated SINKS sub-sections are used. Keyword definitions for input are as follows:

IGEOM	1 for Plane Wall, 2 for Cylindrical Co-ordinates
RHO	Density (kg/m ³)
KHS	Thermal Conductivity (W/m/K)
CPHS	Specific Heat (J/kg/K)
QV	Volumetric Heat Generation (W/m ³)

XRI	Inner Radius (m)
XRO	Outer Radius; for plane walls, outer radius minus inner radius is thickness (m)
AHS	Heat Sink Area (m ²)
TIINIT	Initial inside surface temperature (C)
TOINIT	Initial outside surface temperature (linear profile) (C)
IMSLAB	Number of slabs
IREGI	Region index for inside surface or 0 (insulated) or -1 (constant temperature)
TIHS	Inner surface temperature when IREGI = -1 (C)
IREGO	Region index for outer surface or 0 (insulated) or -1 (constant temperature)
TOHS	Outer surface temperature when IREGO = -1 (C)
XLHS	Characteristic length for natural convection (m)
EHSI	Emissivity of inner surface
EHSO	Emissivity of outer surface
XZHS	Heat sink length (m)

5.2.3.2 Time-Dependent Boundary Conditions

Heat sink surface temperatures can be imposed. Users specify the heat sink number, side number (1 or 2), and two real arrays that impose heat sink temperature as a function of time. The "offset" and extrapolation schemes for imposing region pressure and temperature (defined in the previous section) can also be used for imposing heat sink temperature. A syntax example is as follows:

```
*
* USER CAN CONTROL HEAT SINK BOUNDARY TEMPERATURE
* SYNTAX:
*   OFFSET TIMEHS
*   EXTRAPOLATION TIMEHS
*   TIMTHS IHS ISD TIME1, TIME2...
*   THSFX IHS ISD TEMP1, TEMP2..
* IHS = HEAT SINK NO.; ISD = SIDE NO. (1 OR 2) FOR IHS
* CONTROL HEAT SINK BOUNDARY T
  OFFSET TIMEHS      0.
  EXTRAPOLATION TIMEHS  EXTRAP
  TIMTHS 15 2 0.0      1.E6
  THSFX 15 2 50.0      50.0
  TIMTHS 30 2 0.0      1.E6
```

```

THSFIX 30 2 50.0    50.0
TIMTHS 41 2 0.0    1.E6
THSFIX 41 2 50.0    50.0
TIMTHS 42 1 0.0    1.E6
THSFIX 42 1 50.0    50.0
TIMTHS 42 2 0.0    1.E6
THSFIX 42 2 50.0    50.0

```

5.2.3.3 Material Library

Users can enter heat sink input as shown in Section 5.2.3.1 or opt to use the material library feature, which can facilitate inputs for a large number of heat sinks and decrease the size of the input file. The following material properties can be made part of a library and omitted from the SINKS input: density, thermal conductivity, specific heat, volumetric heat generation rate, inner surface emissivity, and outer surface emissivity. Up to 20 materials can be specified in this way. Syntax is as follows:

```

MATERIAL
  NAME1    INDEX1    RHO    KHS    CP    QV    EHSI    EHSI
  NAME2    INDEX2    RHO    KHS    CP    QV    EHSI    EHSI
END

```

The MATERIAL keyword is a sub-section of the HEAT_SINKS input. An example is as follows:

```

HEAT_SINKS      5      ! Total number of heat sinks
SINKS           1      2      3      4      5
*
IGEOM           0      0      0      0      0
IMATHS          1      1      1      1      1
XRI             0.00610  0.02160  0.00610  0.02160  0.00610
XRO             0.01625  0.03075  0.01625  0.03075  0.01625
AHS             0.278    0.655    0.278    0.655    0.278
XZHS            0.661    0.663    0.661    0.663    0.661
TIINIT          50.00    50.00    50.00    50.00    50.00
TOINIT          50.00    50.00    50.00    50.00    50.00
IMSLAB          3      3      3      3      3
IREGI           3      3      3      3      3
TIHS            0.0      0.0      0.0      0.0      0.0
IREGO           3      3      3      3      3
TOHS            0.0      0.0      0.0      0.0      0.0
XLHS            0.661    0.663    0.661    0.663    0.661

```

END

* MATERIAL LIBRARY - SPECIFY MATERIAL PROPERTIES FOR MATERIAL 'imaths'

* UPTO 20 (INMAT) MATERIALS CAN BE SPECIFIED

* SYNTAX:

* MATERIAL

```

•   name      index      rho      khs      cp      qv      ehsl      ehso
•   END
•   MATERIAL
      URANIUM      1      17102.    26.9    130.    1957.    0.7      0.7
      STSTEEL      2      8000.     16.0    500.     0.      0.25     0.25
      COPPER       3      8954.    398.0   384.     0.      0.7      0.7
      CSTEEL       4      7753.     36.0   486.     0.      0.25     0.25
•   END
•   END HEAT_SINKS ! HEAT_SINKS is a comment

```

5.2.3.4 Composite Heat Sinks

Composite heat sinks, or sandwiches, are heat sinks that consist of two or more layers. In HANSF, consecutive heat sinks can be strung together to make composite heat sinks. Up to 100 composite heat sinks can be created, with up to 10 layers in each wall. Composite heat sinks are constructed so that the outer face of the first heat sink and the inner face of the last heat sink in the series face the gas regions, or are insulated, or have an imposed temperature. Syntax is:

```
SANDWICH HS1 HGAP1 HS2 HGAP2 HS3 HGAP3 ... HSn
```

where SANDWICH is the keyword for a composite heat sink, HS1, HS2, HS3, ..., HSn, are heat sinks defined in the SINKS section, and HGAP is the gap conductance, in W/m²-K, between heat sinks. Gap conductance is often difficult to ascertain and dependent on the nature and extent of contact between heat sink materials. A typical approximation for the gap conductance is $h_{gap} = k_{gap} / \delta$, where k_{gap} is the conductivity of gas in the gap, and δ is the gap thickness.

5.2.3.5 Conduction Networks

Conduction networks can be used to approximate two-dimensional heat transfer, or to model heat sinks that resemble fins, such as the MCO insert and dip tube. A network is specified by the following syntax:

COND_NETWORK HS1, HS2, ... HS_n

The keyword COND_NETWORK is followed by the list of connected heat sinks. In addition to heat transfer at the inner and outer surfaces, heat sinks in the network conduct heat to adjacent heat sinks characterized by the cross-sectional area A_x , the heat sink average temperature T_{avg} , and the axial thickness (XZHS). For each sink, a cross-sectional area, A_x , is equal to the heat sink volume divided by the length (XZHS) and is distinct from the heat transfer surface area, AHS. Heat conduction between two dissimilar material heat sinks and with different cross-sectional areas is handled accurately using the discretization formulation in Section 2.3.1.1.

5.2.3.6 Radiation Networks

Heat sinks can exchange thermal radiation based on heat sink surface area and view factors. Two keywords are used: RAD_NETWORK and FVIEWHS. Syntax is as follows:

```

RAD_NETWORK      HS1, HS2 ... HSn
FVIEWHS          VF11  VF12  VF13... VF1n
                  VF21  VF22  VF23... VF2n
                  .
                  .
                  VFn1  VFn2  VFn3... VFnn

```

where n is the number of heat sinks in the network, and VF_{ij} is the view factor from heat sink i to heat sink j . An example of an enclosure where three surfaces exchange heat by radiation only is shown below:

HEAT_SINKS	3	Total number of heat sinks	
SINKS	1	2	3
* IGEOM	1	1	1
RHO	1000.	1000.	1000.
KHS	20.0	5.0	8.0
CPHS	500.00	500.0	500.0
QV	0.000	0.000	0.000
XRI	0.00000	0.0	0.0
XRO	0.10000	0.1	0.1
AHS	10.0000	15.000	22.000

```

TIINIT      726.85   326.85       26.85
TOINIT      726.85   326.85       26.85
IMSLAB      20       20          20
IREGI       0        0           0
TIHS        0.0      0.0         0.0
IREGO       0        0           0
TOHS        0.0      0.0         0.0
XLHS        1.000    1.0         1.0
XZHS        1.000    1.0         1.0
EHSI        0.9      0.5         1.0
EHSO        0.9      0.5         1.0
END
rad_network  1        2        3
fviewhs     0.0      0.39    0.61
            0.26    0.33    0.41
            0.28    0.28    0.44
*
END HEAT_SINKS ! HEAT_SINKS is a comment

```

5.2.3.7 Temperature-Dependent Emissivity

The user has an option to input a temperature-dependent emissivity. By inputting a negative integer for the emissivity and providing a corresponding temperature versus emissivity look-up table in the heat sink input section, at each time step the code will use the table to determine the emissivity. Up to 20 such look-up tables are allowed and each table can have up to 10 entries.

The key words for the temperature-dependent emissivity look-up table are TTABLE and ETABLE. An example is as follows:

```

TTABLE  2    273.15   373.15   473.15   573.15   673.15
ETABLE  2    0.7      0.65    0.6      0.57    0.53

```

In this case, the emissivity of the heat sink surfaces for which the emissivity is specified as '-2' is determined using above look-up table. Between temperatures, the code interpolates linearly.

5.2.4 JUNCTIONS Section

Syntax for the JUNCTIONS section is as follows:


```

JUNCTIONS      3
*
  PATHS        1      2      3
              Junction Input Keywords
END
*
END

```

The keyword JUNCTIONS is followed by the number of junctions, which is three in this example; a maximum of 10 junctions is allowed. The next keyword PATHS is followed by junction numbers that denote column headings for input values; these numbers must be in order.

Input keywords are listed below:

IJTYP	Junction Type; 1 = Normal, 2 = HEPA, 3 = Cover, 4 = Failure, 5 = Check Valve
IR1	Upstream Region
IR2	Downstream Region
AJN	Area (m ²)
ABYP	Bypass area for HEPA Junction (m ²)
PHEPA	HEPA Filter Failure Pressure (Pa)
ACOV	Cover Area (m ²)
MCOV	Cover Weight (kg)
Z1JN	Elevation with respect to floor of IR1 at IR1 opening (m)
Z2JN	Elevation with respect to floor of IR2 at IR2 opening (m)
CJN	Loss coefficient multiples $\frac{1}{2} \rho * V^2$
IHORIZ	Orientation
XWJN	Characteristic Width (m)
XHJN	Characteristic Height (m)
XLJN	Characteristic Length (m)
DFJN	Decontamination Factor
N90	No. of 90° Bends
IFAN	Fan Type; 0 = Constant Q, 1 = Constant ΔP
WVFAN	Fan Volumetric Flowrate (m ³ /s)

DP1	Opens Failure Junction; Opens Check Valve (Pa)
DP2	Opens Failure Junction, Closes Check Valve (Pa)

The first three types of junctions are: normal, HEPA, and cover. Normal denotes a normally open flowpath. If a HEPA filter is designated, the failure pressure and bypass area must be specified as well. A cover can lift open once a substantial pressure differential is attained, hence the need for a cover weight. Once a type of junction is specified, accompanying values for the other types of junctions are not needed. Variables IHORIZ, XWJN, XHJN, and XLJN are used by the counter-current flow model. IHORIZ = 1 denotes a horizontal wall, i.e., an opening in a floor or ceiling so that flow is vertical. IHORIZ = 0 denotes a vertical wall, i.e., an opening in a wall so that flow is horizontal. XWJN = XHJN denotes a circle. That is, if $|XWJN - XHJN| / XWJN$ is less than or equal to 1.E-4, counter-current flow subroutines evaluate the junction using the expressions for a circle.

Two more junction types are IJTYP = 4 for failure junctions and IJTYP = 5 for check valve junctions. These two types of junctions require two inputs: DP1 and DP2. A failure junction is normally closed. For a failure junction, DP1 is the pressure differential required to fail from the upstream compartment to the downstream compartment. DP2 is the pressure differential required to fail from the downstream compartment to the upstream compartment. Once the junction has failed, it remains open. For a check valve junction, DP1 is the differential pressure required to open the junction from upstream to downstream only. The junction will close when the differential pressure falls below DP2. The time of failure for a failure junction and the cumulative open duration for the check valve junction are printed in the summary part of the output file.

Each junction is allowed to have one fan. The fan can be either a constant volumetric flow fan or a constant pressure differential fan. The junction input parameter IFAN specifies the type of the fan: 0 for constant volumetric flow fan and 1 for constant ΔP fan. For both types, the user inputs the volumetric flow rate of the fan, WVFFAN. For the constant ΔP fan, the volumetric flow rate is converted to the corresponding ΔP at time = 0:

$$\Delta P_{\text{fan}} = \frac{c_j P_{\text{donor}} WVFAN^2}{2 A_j^2} \quad (5-12)$$

where $c_j = C/N_j$, the loss coefficient for junction j . For the constant volumetric flow fan, a safeguard is provided to prevent donor compartment vacuum. The imposed volumetric flow rate of the fan is ramped down when the donor node pressure falls below 10 Pa:

$$WVFAN1 = WVFAN (P_{\text{donor}} / 10 \text{ Pa})^2 \quad (5-13)$$

If the donor pressure falls below 1 Pa, the imposed volumetric flow rate is set to zero.

For the constant ΔP junction, the fan pressure differential is split in half and one half is added to the donor side face pressure of the junction while the other half is subtracted from the receiver side face pressure of the junction. That is,

$$P_{j,\text{donor}} = P_{j,\text{donor}} + P_{\text{fan},j} / 2 \quad (5-14a)$$

and

$$P_{j,\text{receiver}} = P_{j,\text{receiver}} - P_{\text{fan},j} / 2 \quad (5-14b)$$

It should be noted that the counter-current flow is disabled for fan junctions

The user-specified decontamination factor DFJN is defined as:

$$DF = \frac{W_{\text{in}}}{W_{\text{out}}} \quad (5-15)$$

where W_{in} is the aerosol mass flowrate into the junction and W_{out} is the aerosol mass flowrate out the junction. Variable DFJN allows the user to model HEPA filters, or other aerosol deposition mechanisms. Variable N90, the number of 90° bends, is used to model aerosol deposition due to 90° bends, as discussed in Section 2.1.8.

Syntax below shows the input for three normal junctions:

```

*-----
JUNCTIONS    3 1 3 Junctions
*-----
* 1) MCO bottom to MCO middle, 6->5
* 2) MCO middle to MCO top, 5->1
* 3) MCO top to Outlet volume, 1->4
*
* Syntax:
*
*   PATHS      1          2          3
*
*   IJTYP      1          1          1
*   IR1        6          5          1
*   IR2        5          1          4
*   IHORIZ     1          1          1
*   XWJN       0.61       0.61       2.54E-2
*   XHJN       0.61       0.61       2.54E-2
*   XLJN       0.001      0.001      10.
*   AJN        0.29       0.29       0.0
*   Z1JN       1.2        1.2        10.
*   Z2JN       0.0        0.0        12.65
*   CJN        1.0        1.0        4.0
*   DFJN       1.0        1.0        1.0
*   N90        3          3          3
*
*   END PATHS  ! PATHS is a comment.
*
*   END JUNCTIONS ! JUNCTIONS is a comment.

```

5.2.5 MCO Section

This section specifies input to MCO-specific routines that consider the following phenomena: fuel/scrap oxidation, hydriding/dehydriding, heat transfer to the MCO gas space, water evaporation/condensation, aerosol entrainment and de-entrainment, nitriding, and hydrate decomposition. HANSF models the spent fuel as a collection of "tiers", where a tier can be either a fuel assembly or a scrap basket. Up to six tiers are allowed. Users would typically specify one scrap basket, and up to five fuel assemblies.

MCO input contains five sub-sections: GENERAL, SOLAR_RAD, PLOT, FUEL_BSKT, and SCRAP_BSKT. The GENERAL sub-section contains parameters for the following: (1) activating or deactivating specific MCO models, such as oxidation, hydriding, etc., (2) sludge physical properties, such as density, specific area, and particle diameter, (3) coefficients for hydrate decomposition rate laws and decomposition enthalpies, (4) pump flowrate, and (5) radiolysis heat loads.

SOLAR_RAD contains pointers for heat sinks that receive solar radiation, and an array to specify solar radiation as a function of time.

PLOT specifies variables for an MCO-specific plot file, much like the main plot file described in Section 5.2.1.5.

FUEL_BSKT contains parameters to identify which heat sink pairs comprise the fuel basket(s), and which heat sinks represent the MCO wall(s) and lid. For each fuel basket, oxidation areas, free water content, wetted areas, and sludge amounts are specified. A view factor matrix is used to compute thermal radiation exchange between fuel assemblies, the insert, and MCO wall(s). A similar matrix is needed for the micro-convection calculation, which requires the gap distance between fuel assemblies, the insert, and MCO wall(s). Individual fuel baskets can be further subdivided into computational fuel basket cells to consider axial variations in oxidation area, free water content, sludge amounts, etc. This amounts to subdividing a single fuel basket into several fuel basket cells and including the ability to calculate axial conduction heat transfer between cells.

SCRAP_BSKT is much like FUEL_BSKT. It contains general scrap basket dimensions, parameters to define the heat sinks that comprise the scrap basket, including the scrap and copper fin, and pointers for heat transfer to adjacent MCO wall and lid heat sinks. The position of the heat sinks with respect to each other is given for the scrap basket heat transfer, which approximates two-dimensional heat transfer as a series of one-dimensional heat transfer paths. As with the fuel basket(s), oxidation areas, free water content, wetted areas, and sludge amounts are specified. Oxidation and water content are specified on a per unit volume basis. As with the fuel basket, scrap baskets can be further subdivided into computational cells to consider axial variations in oxidation area, free water content, sludge amounts, etc.

5.2.5.1 GENERAL Sub-Section

An example of syntax for the GENERAL sub-section is as follows:

GENERAL ! Keyword for general inputs

IOXDTN 1 ! =1, do oxidation of fuel/scrap
 ! =0, disable oxidation of fuel/scrap

IHYD 0 ! =1, do hydriding/dehydriding calculation
 ! =0, disable hydriding/dehydriding calculation

IDIVRT 3 ! =0, no diversion heat transfer calculation
 ! =1, normal diversion heat transfer calculation
 ! =2, suppress the individual diversion when
 QTDVRT > 0 but Tfi < Tgas, or
 QTDVRT < 0 but Tfi > Tgas
 ! =3, suppress the individual diversion when
 QTDVRT > 0 but Tfi < Tgas

IEVAP 1 ! =1, do evaporation/condensation of water
 ! =0, do not do evaporation/condensation

ILAW 1 ! oxidation rate law, 0 - McGillivray/Ritchie
 ! 1 - Pearce
 2 - Trimble

IDEENT 0 ! =1, de-entrainment of aerosol due to scrap basket
 ! =0, disable de-entrainment calculation

IENTR 0 ! =1, do entrainment of sludge particle calculation
 ! =0, disable entrainment calculation

IHYDKP 1 ! =0, normal depletion of hydride (rate decreases with mass)
 ! =1, use constant hydride reaction area corresponding to
 the initial hydride inventory
 ! =2, use constant reaction area but the area goes to zero
 when all the mass is depleted

INITRI 0 ! =1, do nitriding calculation
 ! =0, disable nitriding calculation

IRADIO 0 ! =1, do radiolysis calculation
 ! =0, disable radiolysis calculation

* XDHYD 2.E-5 ! average diameter of hydride particle (m). this is
 ! overridden by basket specific parameters, XDHYFL & XDHYSC

IHYDKP 0 ! =1, disable depletion of hydride particles
 ! =0, allow hydride particles to disappear as they oxidizes

IHSCSK 42 ! define the cask heat sink

IRGAP 4 ! define the gap node (between MCO wall and the cask)
 ! radiative/convective h.t. between the MCO wall and
 ! cask is computed and some of the heat is diverted
 ! to gas for stability

XGPCSK 0.0155 ! gap distance between the MCO wall and the cask (m)

FHTLID 1.0 ! =0, turn off the radiative heat transfer between the
 ! fuel/scrap and the lid/floor
 ! =1, fully account for the radiative heat transfer

RHOSL 5000. ! sludge particle density (kg/m³)

SASL 1000. ! sludge specific area (m²/m³)

XDSL 1.E-6 ! sludge particle diameter (m)

•

• Hydrate Model: two-step decomposition,
• input curves for ln P and ln K
• first step for x > XHYD2, second step for x < XHYD2
•

• Bounding case: 42 kg particulate, 0.8 kg h₂o = 1.9%

• of sludge being hydrated with 2 moles of
• water per mole of uranium oxide
•

FHYSL 0.1732 ! fraction of sludge that is hydrated

XHYSL 2.0 ! stoichiometry number of hydrate: no. of moles of
 ! water per mole of uranium oxide (UO₃.H₂O)

XHYD2 1.0 ! H₂O/U ratio (stoich. number) to switch
 ! from first to second correlation

XHYD3 0.5 ! H₂O/U ratio (stoich. number) to switch
 ! from second to third correlation

*

```

AHYEQ1 15.912 ! 'A' IN LN P = A + B/T FOR X > XHYD2
BHYEQ1 -6131.E0 ! 'B' IN LN P = A + B/T FOR X > XHYD2
AHYEQ2 18.382 ! 'A' IN LN P = A + B/T FOR X < XHYD2
BHYEQ2 -7766.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD2
AHYEQ3 18.408 ! 'A' IN LN P = A + B/T FOR X < XHYD3
BHYEQ3 -8488.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD3
*
ADEHY1 2.793E0 ! 'A' IN LN K = A + B/T FOR X < XHYD2
BDEHY1 -5111.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD2
ADEHY2 6.348E0 ! 'A' IN LN K = A + B/T FOR X > XHYD2
BDEHY2 -7241.E0 ! 'B' IN LN K = A + B/T FOR X > XHYD2
ADEHY3 4.632E0 ! 'A' IN LN K = A + B/T FOR X < XHYD3
BDEHY3 -7548.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD3
*
DHHY1 2.86E6 ! Decomposition enthalpy J/kg H2O: 1st step
DHHY2 3.70E6 ! Decomposition enthalpy J/kg H2O: 2nd step
DHHY3 3.70E6 ! Decomposition enthalpy J/kg H2O: 3rd step
FPROHY 1.0 ! hydride production rate law multiplier
FCONHY 1.0 ! hydride consumption rate law multiplier
FNITRI 1.0 ! nitriding rate law multiplier
FO2HYH2 0.0 ! fraction of O2 reacting with uranium hydride which
! produces hydrogen instead of steam
*
* PUMP, FEED, AND CONDENSER MODELS
* Syntax:
* PUMP IRIPUM IROPUM ICONPM ITFEED WVPUMP WVFEED TGFEED TCONPM
*
* Definitions:
* IRIPUM - Pump inlet region
* IROPUM - Pump outlet region
* ICONPM - Node to which the condensed steam is dumped for book-keeping
* ITFEED - If non-zero, overrides TGFEED with the designated region
* temperature. Used to specified time-varying feed temperature
* WVPUMP - Pump volumetric flowrate (m^3/s)
* WVFEED - Feed volumetric flowrate (m^3/s)
* TGFEED - Feed temperature (C)
* TCONPM - Condenser cooling coil temperature (C)
*
* 35 FT^3/MIN * 1 MIN/60 SEC * 0.02832 M^3/1 FT^3 = 0.01652 M^3/SEC
* PUMP IRIPUM IROPUM ICONPM ITFEED WVPUMP WVFEED TGFEED TCONPM
PUMP 1 5 0 0 1.652E-2 0.0 0.0 0.0
*
* Radiolysis parameters
*
FRAD 1.0 ! multiplier for radiolysis
FALPHA 0.197 ! alpha fractional heat load
FBETA 0.486 ! beta fractional heat load
FGAMMA 0.317 ! gamma fractional heat load
QPHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
! per MTU of fuel loading
END GENERAL ! GENERAL is a comment
*

```

The first ten input variables simply toggle MCO phenomenological models. For all these variables, except ILAW, an integer value of 0 switches the model to "off"; although any real or integer value other than 0 can switch the model "on", an integer value of 1 is recommended. ILAW must be an integer value of either 0 or 1. This sub-section contains obvious sludge properties such as average particle size, XDSL (m), particle density, RHOSL (kg/m³), and the

fraction of sludge that is hydrated, FHYSL. Sludge-specific area, SASL, is defined as the sludge area divided by sludge mass. The stoichiometry of the hydrate (XYHSL, XHYD2, and XHYD1) is simply the number of moles of water per mole of uranium oxide, e.g., for $\text{UO}_2 \cdot 2\text{H}_2\text{O}$, XHSYL = 2. Rate law multipliers are included for hydride production, hydride consumption, and nitriding (FPROHY, FCONHY, and FNITRI, respectively). Parameters for the hydrate model are described in Section 3.5.

A pump model takes suction from an inlet node (IRIPUM) and forces a specified volumetric flowrate (WVPUMP) into an outlet node (IROPUM). Only one such pump is allowed, but it can be combined with non-mechanistic condenser and re-heater models as described below. Pump flowrate is limited so that the inlet node pressure does not fall below 1 torr (133 Pa) during a time step.

Simple condenser and re-heater models are required for recirculation mode operations. The condenser model works in conjunction with the pump flow model; i.e., the volumetric flowrate from the pump passes through the condenser. The condenser model is based on a user-specified condenser cooling coil temperature, TCONPM. It is activated if the user-specified condenser cooling coil temperature (TCONPM) is greater than 273.15 K. Steam partial pressure in the gas flow is reduced to the saturation pressure for TCONPM. The fraction of steam flow condensed, f , is then:

$$f = 1.0 - \text{Min} \left(1.0, \frac{P_c}{P_{st}} \right) \quad (5-16)$$

where Min is the minimum function, P_c is the saturation pressure at TCONPM, and P_{st} is the steam flow partial pressure. The re-heater model then adjusts the enthalpy of the gas entering the outlet node to match the user-specified feed temperature set-point (TGFEED), if desired. Otherwise, the gas enthalpy is set to that of the inlet (or donor) node. A user-specified helium volumetric flowrate, WVFEED, can be added to the flow entering the outlet node. The helium enthalpy is set to the user-specified feed temperature, TGFEED.

The last five variables are used by the radiolysis model described in Section 3.10. FRAD is a multiplier that can be used to account for local variations in heat loading. FALPHA, FBETA, and FGAMMA are fractional heat loads for alpha, beta, and gamma radiation, respectively. These values must sum to 1.0. The values shown here are from [Pajunen, 1997]. QPHOTO is the heat deposition rate in MCO free water per gram per MTU of fuel loading.

5.2.5.2 SOLAR RADIATION Sub-Section

An example of this sub-section is shown below:

```

SOLAR_RAD
*
* pointers to heat sinks representing the cask wall and the top
* solar radiation impinges on these
*
  IHCASK  42
  IHTOP   44
*
* look-up table for solar radiation throughout a day (sec .vs. W/m^2)
*
  OFFSET_TIMDAY      21600.  ! offset by six hours
  EXTRAPOLATION_TIMDAY PERIOD ! repeat the diurnal cycle
  TIMDAY      0.0  3600.0  7200.0 10800.0 14400.0 18000.0 21600.0
              25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
              50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
              75600.0 79200.0 82800.0 86400.0
  RADSUN      0.0    0.0    0.0    0.0    0.0    5.5    21.2
              47.9    79.1   108.0  131.3  147.7  155.9  155.5
              146.7   130.9   108.0   80.8   51.1   24.4    6.3
              0.0    0.0    0.0    0.0
END SOLAR_RAD
*
```

The offset feature can be used to start the run at any point in diurnal cycle, and the PERIOD extrapolation feature can repeat the diurnal cycle if the run lasts more than 24 hours. Input variables IHCASK and IHTOP specify the heat sinks that receive solar radiation. TIMDAY must be in seconds, and RADSUN must be in W/m^2 .

5.2.5.3 FUEL_BSKT Sub-Section

A sample of fuel basket input is shown below:

```

FUEL_BSKT  4  ! Total number of fuel baskets
*
* 1st Fuel Basket
*
* heat sink pairs for fuel basket #1
*
IHSFPL  46 47 48 49 50 51 52 53 54 55 56 57 58 59
IFLINS  81      ! define the adjacent center insert heat sink,
                ! 0 for no insert
IFLMCO  60      ! define the adjacent MCO wall heat sink
IFLLID  0      ! define the lid or floor heat sink to which the fuel
                ! radiate to
AFLFL  0.131    ! flow area in the basket,
*
* fraction of geometric area exposed for oxidation
*  $3.5 \text{ m}^2 / (4 \times 16.8 \text{ m}^2) = 0.0521$ 
FAOXFL  0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521
        0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521
FOX      10 0    ! multiplier for FAOXFL
XDHYFL  2.E-5    ! average diameter of hydride particle (m)
*
* Nominal hydride: 4% of exposed surface with multiplier of 300
*  $\text{XFLOX0} \cdot \text{FXHD0} = \text{Fx} \cdot \text{Fa} \cdot \text{XDHYD} / 6$ , where Fx is multiplier
                and Fa is area fraction
*
*  $= 0.04 \cdot 300 \cdot 2.E-5 / 6$ 
*
*  $= 4.0E-5$ 
*
* XFLOX0: initial oxide (oxide+hydride) thickness
* (to be applied to exposed area)
*
* FXHYD0: fraction of initial oxide which is hydride
*
XFLOX0  4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
        4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
FXHYD0  1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
        1.0 1.0 1.0 1.0 1.0 1.0 1.0
*
* initial amount (kg) of water per geometric surface area ( $\text{m}^2$ ) of fuel
*  $0.1 \text{ kg} / 16.8 \text{ m}^2 = 0.0060$ 
FWFL0  0.0060 0.0060 0.0060 0.0060 0.0060 0.0060 0.0060 0.0060
        0.0060 0.0060 0.0060 0.0060 0.0060 0.0060 0.0060
FWFLI0  0.0    ! on the outer surface of the insert
FWFLM0  0.0    ! on the inner surface of the MCO wall
FAWFL  0.1    ! wetted fraction of fuel surface
FAWFLM  1.0    ! wetted fraction of MCO wall
MSLFL  5.2    ! mass of sludge particles (kg) in the fuel basket
                ! 20.8 total fuel @ 4 baskets, so 5.2 per basket
*
* view factor matrix between the insert,
* outer surface of outer fuel elements,
* and the MCO wall. Therefore, the dimension of the square matrix is
*  $1 + \text{number of fuel rods} + 1$ . If there is no insert, number of fuel rods + 1.
*
FVIEW  0.000 0.926 0.074 0.000 0.000 0.000 0.000 0.000 0.000
        0.175 0.316 0.306 0.181 0.028 0.000 0.000 0.000 0.000
        0.014 0.306 0.028 0.306 0.306 0.028 0.014 0.000 0.000
        0.000 0.181 0.306 0.000 0.334 0.153 0.000 0.028 0.000
        0.000 0.014 0.153 0.167 0.167 0.153 0.153 0.167 0.028

```

0.000	0.000	0.028	0.153	0.306	0.000	0.028	0.306	0.181
0.000	0.000	0.014	0.000	0.306	0.028	0.000	0.306	0.348
0.000	0.000	0.000	0.014	0.167	0.153	0.153	0.049	0.466
0.000	0.000	0.000	0.000	0.035	0.115	0.220	0.590	0.040

*
 * gap distance for micro-convection calculation
 *
 XGAP 0.000 0.018 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 0.018 0.000 0.021 0.021 0.073 0.000 0.000 0.000 0.000
 0.000 0.021 0.000 0.021 0.021 0.073 0.073 0.000 0.000
 0.000 0.021 0.021 0.000 0.021 0.021 0.000 0.073 0.000
 0.000 0.073 0.021 0.021 0.000 0.021 0.021 0.021 0.083
 0.000 0.000 0.073 0.021 0.021 0.000 0.073 0.021 0.058
 0.000 0.000 0.073 0.000 0.021 0.073 0.000 0.021 0.026
 0.000 0.000 0.000 0.073 0.021 0.021 0.021 0.000 0.016
 0.000 0.000 0.000 0.000 0.083 0.058 0.026 0.016 0.000

*
 * axial conduction tracked in the fuel elements
 *
 * top to bottom axial partitions of the basket
 AXIAL 0.0521 0.0425 0.0648 0.0995 0.152 0.234 0.3551
 * multiplier to FAOXFL(fraction of geometric area exposed for
 * oxidation) for each axial basket. clad damage confined to the tip.
 * 1./0.0521=19.19
 FOXAX 19.19 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * multiplier to FWFL0, FWFL10, and FWFM0 (initial amount of water per
 * geometric surface area of fuel, insert, and MCO wall) for each axial
 * basket. water on the tip of fuel. 1./0.0521=19.19
 FWAX 19.19 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * multiplier to XFLOX0 (initial oxide/hydride thickness) for each axial basket
 FUH3AX 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * partition of MSLFL(mass of sludge particles) for each axial basket. uniform.
 FSLAX 0.0521 0.0425 0.0648 0.0995 0.152 0.234 0.3551
 END IHSFL for 1st fuel basket

The keyword FUEL_BSKT is followed by the number of fuel baskets to be modeled. The sum of the number of fuel baskets and the number of scrap baskets must be less than six. Typically, the user will be interested in modeling one scrap basket, and up to five fuel baskets. Fuel basket input allows the user to account for differences between fuel baskets in one MCO. If there are no differences, then only one set of fuel basket input is necessary, provided that the input reflects the fact that there are four fuel baskets. To model more than one fuel basket, the FUEL_BSKT sub-section is repeated for each fuel basket.

Many parameters are the same for all fuel baskets. To minimize input, a keyword "SAME AS FUEL BASKET n", where n is an integer designator for a previously defined fuel basket, may be used. Upon encountering this key word, HANSF will copy all inputs from fuel basket n to the current fuel basket input. Any differing input parameter values can be placed on subsequent lines. HANSF will over-write the old values with the new values. For example:

```

*
* 2nd Fuel Basket
*
  SAME AS FUEL BASKET 1
  IHSFL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
  IFLMCO 30
  IFLFLID 43
  END IHSFL for 2nd fuel basket

```

This syntax can be used to create a second fuel basket that has the same input as FUEL BASKET 1, except for IHSFL, IFLMCO, and IFLFLID.

IHSFL defines the heat sink pairs that make up the fuel basket. Each successive pair of values gives the heat sink numbers that correspond to the inner and outer fuel elements of the fuel assembly. The sample above gives the input for the nodalization shown in Figure 3-7. Pointers include IFLMCO, which specifies the adjacent MCO wall heat sink, IFLFLID, which specifies the MCO floor or lid that the fuel basket radiates to, and IFLINS, which specifies the adjacent center-insert heat sink. If there is no adjacent floor, lid, or insert, zero is specified as the pointer for that heat sink. The flow area in the basket, AFLFL, would nominally be equal to the cross-sectional area of the MCO minus the cross-sectional area of the 54 fuel elements.

Each heat sink listed as an IHSFL value requires a value for FAOXFL - the "geometric surface area." Geometric surface area is expressed as a fraction of the actual heat sink; if FAOXFL = 1.0, the geometric surface area is simply equal to the heat sink area. FOX, a multiplier for FAOXFL, takes into account uncertainties in the actual oxidation reaction area and can be used to specify any desired oxidation reaction area. FOX has two values because it is a temperature-dependent multiplier, with the functional form of

$$\text{FOX} = \max \left(1, f_1 f_2 10^{\left(\frac{f_2}{T} \right)} \right) \quad (5-17)$$

where f_1 is the first parameter value, f_2 is the second, and T is the heat sink temperature in K. The user can develop custom, temperature-dependent oxidation rate laws by choosing the parameter values for FOX appropriately. For hydriding and nitriding reactions, the geometric surface area is multiplied by rate law multipliers to obtain the final reaction rate.

XDHYFL represents the average diameter of hydride particles on the fuel. It is used to determine the hydride oxidation area.

FWFLO, FWFLI, and FWFLMO all express initial water inventory in terms of kg per geometric surface area. There must be a one-to-one correspondence between the number of FWFLO values and the number of IHSFL values. FAWFL and FAWFLM allow the user to specify the area fraction of fuel sludge and MCO wall, respectively, that participate in evaporation and condensation, so as to model an uneven distribution of water.

If there is an insert (IFLINS is non-zero), then the view factor matrix has dimensions $(1 + NA + 1) \times (1 + NA + 1)$, where NA is the number of fuel assemblies. If there is no insert (IFLINS equals zero), the view factor matrix has dimensions $(NA + 1) \times (NA + 1)$.

		Insert	Fuel Assembly #							MCO Wall
			1	2	3	4	5	6	7	
Insert		0.000	0.926	0.074	0.000	0.000	0.000	0.000	0.000	0.000
Fuel Assembly #	1	0.175	0.316	0.306	0.181	0.028	0.000	0.000	0.000	0.000
	2	0.014	0.306	0.028	0.306	0.306	0.028	0.014	0.000	0.000
	3	0.000	0.181	0.306	0.000	0.334	0.153	0.000	0.028	0.000
	4	0.000	0.014	0.153	0.167	0.167	0.153	0.153	0.167	0.028
	5	0.000	0.000	0.028	0.153	0.306	0.000	0.028	0.306	0.181
	6	0.000	0.000	0.014	0.000	0.306	0.028	0.000	0.306	0.348
	7	0.000	0.000	0.000	0.014	0.167	0.153	0.153	0.049	0.466
MCO Wall		0.000	0.000	0.000	0.000	0.035	0.115	0.220	0.590	0.040

If there is an insert:

- The first row/column of the matrix represents the outer surface of the insert,

- The second row/column of the matrix represents the outer surface of the outer element of the first fuel assembly, as listed in the IHSFL input parameter array,
- The third row/column represents the outer surface of the second fuel assembly as listed in the IHSFL input parameter array, and so on, and
- The last row/column represents the MCO wall.

If there is no insert,

- The first row/column of the matrix represents the outer surface of the outer element of the first fuel assembly, as listed in the IHSFL input parameter array,
- The second row/column represents the outer surface of the second fuel assembly as listed in the IHSFL input parameter array, and so on, and
- The last row/column represents the MCO wall.

Although Section 1.11 concludes that axial variations may be neglected as a reasonable approximation, HANSF includes the capability of modeling axial variations in fuel baskets. This is accomplished by subdividing a fuel basket into a number of "fuel basket cells" so that each cell represents an axial segment of the real fuel basket. Fuel basket cells can conduct heat axially to one another, and can have unique reactive areas, hydride contents, sludge masses, and water contents.

Adding the following lines to the fuel basket input creates fuel basket cells:

```
*
* axial conduction tracked in the fuel elements
*
* top to bottom axial partitions of the basket
AXIAL 0.0521 0.0425 0.0648 0.0995 0.152 0.234 0.3551
* multiplier to FAOXFL(fraction of geometric area exposed for
* oxidation) for each axial basket. clad damage confined to the tip.
* 1./0.0521=19.19
FOXAX 19.19 0.0 0.0 0.0 0.0 0.0 0.0
* multiplier to FWFL0, FWFLI0, and FWFM0 (initial amount of water per
* geometric surface area of fuel, insert, and MCO wall) for each axial
* basket. water on the tip of fuel. 1./0.0521=19.19
FWAX 19.19 0.0 0.0 0.0 0.0 0.0 0.0
```

* multiplier to XFLOX0 (initial oxide/hydride thickness) for each axial basket
 FUH3AX 1.0 0.0 0.0 0.0 0.0 0.0 0.0
 * partition of MSLFL(mass of sludge particles) for each axial basket. uniform.
 FSLAX 0.0521 0.0425 0.0648 0.0995 0.152 0.234 0.3551
 END IHSFL for 1st fuel basket

Keyword AXIAL creates a set of cells representing axial segments of the first fuel basket, according to the listed partitioning. Seven axial segments are created here, and the seven partition fractions must sum to one. Note that the spacing is tighter near the damaged end, so as to capture temperature gradients with a minimum number of cells. FOXAX specifies distribution of damaged area. In this example, all the damage is at one end, which means if the damaged end is 5.21% of the height (about 3.5 cm) the multiplier is $1.0 / 0.0521 = 19.19$ for the first cell and zero for the other six cells. Similar logic applies to FWAX, which specifies the distribution of surface water mass. FUH3AX is a multiplier to XFLOX0 and can be used to distribute the initial hydride mass in any manner. FSLAX shows partition fractions for the sludge mass. As with the AXIAL partition, the partition fractions in FSLAX must sum to 1.0.

HANSF will generate additional heat sink and fuel basket inputs based on the input for the AXIAL keyword. Seven fuel baskets segments are strung together for axial conduction, as follows:

	Fuel Heat Sinks																	MCO wall
Segment 1:	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60			
Segment 2:	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89			
Segment 3:	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104			
Segment 4:	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119			
Segment 5:	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134			
Segment 6:	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149			
Segment 7:	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164			

Thus, the code will generate 90 additional heat sinks and 6 additional fuel basket cells, and assign appropriate inputs for them. Also, the surface area, reactive area, and water mass will be appropriately adjusted for heat sinks 46 through 60. Heat transfer due to axial conduction has to be calculated for an axially connected set of heat sinks; e.g., between heat sinks 46, 75, 90, 105, 120, 135, and 150. The sequence of heat sinks over which conduction must be calculated, and the corresponding heat sink dimensions and properties, are set up before calling AXCOND to do conduction calculation.

5.2.5.4 SCRAP_BSKT Sub-Section

A maximum of two scrap baskets is allowed. An example of scrap basket input is as follows:

```

SCRAP_BSKT 1      ! Total number of scrap baskets
*
* First scrap basket
*
IHSSC  61 70 63 64 65 66 67 68 69      ! radial outward
*
ISCINS 83      ! define the adjacent center insert heat sink,
               ! 0 for no insert
ISCFIN 62      ! define copper fin heat sink
ISCMCO 71      ! define the adjacent MCO wall heat sink
ISCLID 74      ! define the lid or floor heat sink to which the scrap
               ! radiate to
* multiplier for effective conductivity in scrap basket in the order read in
* (only conduction part)
FKSC 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
* multiplier for effective conductivity in scrap basket in the order read in
* (only radiation part)
FRSC 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
* porosity of the scrap for each heat sink in the order read in
FPOROS 0.40 0.40 0.40
        0.685 0.685 0.685 0.685 0.685 0.685
* characteristic size for each scrap heat sink in the order read in (m)
XDSCRP 0.00635 0.00635 0.00635
        0.0254 0.0254 0.0254 0.0254 0.0254 0.0254
XRSCBK 0.2842 ! radius of scrap basket (m)
XHSCBK 0.676 ! height of scrap basket (m)
*
* exposed surface area available for oxidation
* per unit volume of scrap (1/m) for
* each scrap basket heat sink in the order read in
* Fine: Area= 2.5 m^2 Volume= 1.59e-2 m^3 A/V=157.2
* Coarse: Area= 2.0 m^2 Volume= 1.517e-1 m^3 A/V=13.18
AVOXSC 157.2 157.2 157.2
        13.18 13.18 13.18 13.18 13.18 13.18
FOXSC 10 0 ! multiplier for AVOXSC
XDHYSC 2.E-5 ! average diameter of hydride particle (m)
*
* Nominal hydride: 4% of exposed surface with multiplier of 300
* XSCOX0*FSCHD = Fx * Fa * XDHYD / 6, where Fx is multiplier
* and Fa is area fraction
* = 0.04 * 300 * 2.E-5 / 6
* = 4.0E-5
* XSCOX0 initial oxide thickness on the exposed surface (m)
* FSCHYD fraction of oxide which is hydride
* see fuel basket
XSCOX0 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
        4.0E-5 4.0E-5 4.0E-5
FSCHYD 1.0 1.0 1.0 1.0 1.0 1.0
        1.0 1.0 1.0
*
* 1.5 kg of water total for scrap basket; 1.5/0.1676 = 8.950 kg/m^3
MWWSC0 8.950 ! initial amount (kg) of water per unit bulk volume
           ! (m^3) of scrap
FWSCIO 0.0 ! on the outer surface of the insert
           ! (per unit area, m^2)

```



```

FWSCMO 0.0      ! on the inner surface of the MCO wall
              ! (per unit area, m^2)
FAWSC  0.1      ! wetted fraction of surface area
FAWSCM 1.0      ! wetted fraction of MCO wall
XSCINS 0.01     ! gap distance between the insert and scrap basket
              ! 1/4" gap for scrap basket and mco wall
XSCMCO 0.00635  ! gap distance between scrap basket and MCO wall
MSLSC  21.2     ! mass of sludge particles (kg) in the scrap basket
*
* axial conduction tracked in the scrap basket, water on the bottom
* 4 nodes, one 2" node at the bottom
*
* top to bottom axial partition
  AXIAL 0.3083 0.3083 0.3083 0.0751
* multiplier for FFOROS(porosity of scrap) for each axial basket
  FFOR 1.0      1.0      1.0      1.0
* multiplier for FOXSC(multiplier for oxidation area) for each axial basket
  FFOXSC 1.0    1.0    1.0    1.0
* multiplier for MVWSC0(initial amount of water per unit volume) for each
* axial basket. 1 kg on the bottom node, 0.167 kg on each of top three nodes.
  FMVWSC 0.3605 0.3605 0.3605 8.877
* multiplier for XDSCR(characteristic scrap size) for each axial basket
  FXDSCR 1.0    1.0    1.0    1.0
* multiplier for FKSC(multiplier for effective conductivity (conduction)
* in scrap)
  FFKSC 1.0      1.0      1.0      1.0
* multiplier for FRSC(multiplier for effective conductivity (radiation)
* in scrap)
  FFRSC 1.0      1.0      1.0      1.0
END IHSSC for 1st scrap basket
END SCRAP_BSKT

```

IHSSC is a matrix of scrap basket heat sinks. The very first heat sink specified is adjacent to the center insert, if present, while the last heat sink specified is adjacent to the copper fin nearest to the MCO wall. Each row of the matrix represents consecutive heat sinks. The first heat sink inside boundary in the row is insulated, and the last heat sink outside boundary in the row is adjacent to the copper fin. For the configuration shown in Figure 3-8, IHSSC would be:

```

IHSSC  67  70  63  64  65  66  67  68  69

```

ISCINS, ISCFIN, ISCMCO and ISCLID are pointers for the heat sinks corresponding to the insert, copper fin, MCO wall adjacent to the scrap basket, and the lid/floor that the scrap basket radiates to, respectively. If any of these is not present, the pointer is set to zero.

FKSC and FRSC are multipliers for effective conductivities in the scrap basket, one for conduction part and the other for radiation part, respectively.

FPOROS, XDSCRCP and AVOXSC each describe the scrap and each must be read in the order specified by IHSSC. XDSCRCP is a characteristic size of the scrap, in meters. Note in the example that the first five heat sink nodes are fine scrap, as evidenced by the lower porosity and smaller characteristic size. AVOXSC is the exposed surface area available for oxidation per unit volume, and has units of 1/m. FOXSC is a temperature-dependent multiplier for AVOXSC, and has the same format as FOX has for the fuel basket. XDHYSK is the average diameter of hydride particles in the scrap basket.

XSCOX0 and FSCHYD describe the hydride content. Consider the example where hydride occupies 4% of the exposed surface and a multiplier of 300 applies. The product of the initial oxide thickness (XSCOX0) and fraction of oxide which is hydride (FSCHYD), can be expressed as follows:

$$XSCOX0 \cdot FXCHYD = F_x F_a \frac{XDHYSK}{6} \quad (5-18)$$

where F_x is the multiplier (300), F_a is the area fraction (4%), and XDHYSK is the hydride particle diameter specified.

HANSF has a capability to consider axial variations in the scrap basket, much like the capability available for axial conduction in fuel baskets. The scrap basket is divided into computational cells that consider axial segments of scrap. HANSF considers axial conduction and axial variations in porosity, oxidation area, water content per unit volume, scrap size, and effective conductivity in the scrap. The following is an example of the syntax to create four axial cells in the fuel basket:

```

*
* axial conduction tracked in the scrap basket, water on the bottom
* 4 nodes, one 2" node at the bottom
*
* top to bottom axial partition
  AXIAL 0.3083 0.3083 0.3083 0.0751

```

```

* multiplier for FPOROS(porosity of scrap) for each axial basket
  FFPOR 1.0 1.0 1.0 1.0
* multiplier for FOXSC(multiplier for oxidation area) for each axial basket
  FFOXSC 1.0 1.0 1.0 1.0
* multiplier for MVWSC0(initial amount of water per unit volume) for each
* axial basket. 1 kg on the bottom node, 0.167 kg on each of top three nodes.
  FMVWSC 0.3605 0.3605 0.3605 8.877
* multiplier for XDSRC(characteristic scrap size) for each axial basket
  FXDSC 1.0 1.0 1.0 1.0
* multiplier for FKSC and FRSC(multiplier for effective conductivity in scrap)
  FFKSC 1.0 1.0 1.0 1.0
  FFRSC 1.0 1.0 1.0 1.0
  END IHSSC for 1st scrap basket
END SCRAP_BSKT

```

Keyword AXIAL is followed by the partition fractions for the scrap, which must sum to one. Other keywords for axial variations in the scrap are:

- FFPOR is the keyword for the axial multiplier for FPOROS, scrap porosity,
- FFOXSC is the axial multiplier for FOXSC, which is itself a multiplier for oxidation area,
- FMVWSC is the axial multiplier for MVWSC0, initial amount of water per unit volume,
- FXDSC is the axial multiplier characteristic scrap size,
- FFKSC is the axial multiplier for effective conductivity in the scrap (conduction), and
- FFRSC is the axial multiplier for effective conductivity in the scrap (radiation).

5.2.5.5 MCO Plotting Sub-Section

The MCO section of the input deck also contains a plotting section that is similar in syntax to the main plotting section, but with variables limited to MCO-specific phenomena. MCO plot variables are as follows:

- PUMPH2 : hydrogen pumping flowrate, kg/s,
- GAS-WH2 n j1, j2, ..., jn : hydrogen flowrate through junctions 1, 2, 3, ..., n, kg/s
- CORRODH2: hydrogen generation rate by corrosion, kg/s
- HS-H2O n hsl, hs2, ..., hsn : mass of water on heat sinks 1, 2, 3, ..., n, kg,
- HS-HYH2O n hsl, hs2, ..., hsn : mass of sludge on heat sinks 1, 2, 3, ..., n, kg,
- QDECFL : decay heat in fuel baskets, W,

- QDECSC : decay heat in scrap baskets, W,
- QDECTT : total decay heat, W,
- UDECTT : integrated decay heat, J,
- QOXOFL : oxidation power in fuel baskets from oxygen, W,
- QOXOSC : oxidation power in scrap baskets from oxygen, W,
- QOXOTT : total oxidation power from oxygen, W,
- UOXOTT : integrated oxidation power from oxygen, J,
- QOXWFL : oxidation power in fuel baskets from water, W,
- QOXWSC : oxidation power in scrap baskets from water, W,
- QOXWTT : total oxidation power from water, W,
- UOXWTT : integrated oxidation power from water, J,
- QNTRFL : nitriding power in fuel baskets, W,
- QNTRSC : nitriding power in scrap, W,
- QNTRTT : total nitriding power, W,
- UNTRTT : integrated nitriding power, J,
- QHYDFL : hydriding power in fuel baskets, W,
- QHYDSC : hydriding power in scrap baskets, W,
- QHYDTT : total hydriding power, W,
- UHYDTT : integrated hydriding power, J,
- QINFL : total power sources in fuel baskets, W,
- QINSC : total power sources in scrap baskets, W,
- QINTT : total power sources, W,
- UINTT : integrated total power sources, J,
- QMCOFL : heat losses from fuel baskets to MCO wall, W,
- QMCOSC : heat losses from scrap baskets to MCO wall, W,
- QMCOTT : total heat losses to MCO wall, W,
- UMCOTT : integrated total heat losses to MCO wall, J,
- QLIDFL : heat losses from fuel baskets to MCO lid/bottom, W,
- QLIDSC : heat losses from scrap baskets to MCO lid/bottom, W,
- QLIDTT : total heat losses to MCO lid/bottom, W,
- ULIDTT : integrated total heat losses to MCO lid/bottom, J,

- QGASFL : heat losses from fuel baskets to gas, W,
- QGASSC : heat losses from scrap baskets to gas, W,
- QGASTT : total heat losses to gas, W,
- UGASTT : integrated total heat losses to gas, J,
- QEVPFL : total heat losses from fuel baskets by evaporation, W,
- QEVPSC : total heat losses from scrap baskets by evaporation, W,
- QEVPTT : total heat losses by evaporation, W,
- UEVPTT : integrated total heat losses by evaporation, J,
- QCNDFL : heat losses from fuel baskets by conduction, W,
- QCNDSC : heat losses from scrap baskets by conduction, W,
- QCNDTT : total heat losses by conduction, W,
- UCNDTT : integrated heat losses by conduction, J,
- QOUTFL : total heat losses from fuel baskets, W,
- QOUTSC : total heat losses from scrap baskets, W,
- QOUTTT : total heat losses from fuel and scrap, W,
- UOUTTT : integrated total heat losses from fuel and scrap, J,
- UMCO : total internal energy of fuel, scrap and water on fuel/scrap, J,
- UINTGT : $UMCO0 + UINTT - UOUTTT$, J, where $UMCO0$ is the total initial internal energy of fuel, scrap, and water on fuel/scrap,
- FUERR : $(UINTGT - UMCO) / UMCO$, -, and
- TOTUO2 : total UO_2 mass in MCO, kg.

An example of syntax for this sub-section follows:

```

PLOT      ! Keyword for MCO-specific plotting section
          ! A plot file with the name 'input deck name'.PL1 is generated
• Plotting syntax:
•
* PUMPH2      - Hydrogen flow rate into the vacuum pump, kg/s
* GAS-WH2 n jlist - Hydrogen flow rate through junctions, kg/s
* CORRODH2    - Hydrogen generation rate by fuel/scrap corrosion
* HS-H2O n hlist - Water mass on heat sink surfaces, kg
* HS-HYH2O n hlist - Water mass in sludge on heat sink surfaces, kg
* WH2F1 n flist  - Hydrogen generation rate by corrosion/dehydriding/
                  radiolysis in fuel baskets, kg/s
•
* WH2SC n slist  - " in scrap baskets, kg/s
* WH2TT        - total hydrogen generation by corrosion/dehydriding/
                  radiolysis in MCO, kg/s
* MH2TT        - cumulative hydrogen generated in MCO, kg
•

```

* QDECFL n flist - decay heat in fuel baskets, W
 * QDECSC n slist - decay heat in scrap baskets, W
 * QDECTT - total decay heat in MCO, W
 * UDECTT - cumulative decay heat in MCO, J
 *
 * QOXOFL, QOXOSC, QOXOTT, UOXOTT fuel corrosion by O2 heat
 * QOXWFL, QOXWSC, QOXWTT, UOXWTT fuel corrosion by H2O heat
 * QNTRFL, QNTRSC, QNTRTT, UNTRTT nitriding heat
 * QHYDFL, QHYDSC, QHYDTT, UHYDTT hydriding/dehydriding heat
 * QINFL, QINSC, QINTT, UINTT total energy in
 *
 * QMCOFL, QMCOSC, QMCOTT, UMCOTT heat loss to MCO wall
 * QLIDFL, QLIDSC, QLIDTT, ULIDTT heat loss to lid/floor/insert
 * QGASFL, QGASSC, QGASTT, UGASTT heat loss to gas
 * QEVDFL, QEVDFSC, QEVPTT, UEVPTT heat loss due to evaporation
 * QCNDFL, QCNDSC, QCNDTT, UCNDTT heat loss by axial conduction
 * QOUTFL, QOUTSC, QOUTTT, UOUTTT total energy out
 *
 * UMCO - total energy in fuel
 * UINTGT - initial energy in fuel + integrated(source-sink)
 * FUERR - relative energy imbalance
 * TOTUO2 - total UO2 in MCO
 *
 * Note: plot routine can only accept 99 items; can't plot all things.
 * So plot all scrap T's but only 5 fuel (plus MCO)
 * jlist - junction list
 * hlist - heat sink list
 * flist - fuel basket list
 * slist - scrap basket list
 *

CORRODH2
 WR2TT
 MR2TT
 QDECFL 1 1
 QDECSC 1 1
 QDECTT
 UDECTT
 QOXOFL 1 1
 QOXOSC 1 1
 QOXOTT
 UOXOTT
 QOXWFL 1 1
 QOXWSC 1 1
 QOXWTT
 UOXWTT
 QINTT
 UINTT
 QMCOFL 1 1
 QMCOSC 1 1
 QMCOTT
 UMCOTT
 QLIDFL 1 1
 QLIDSC 1 1
 QLIDTT
 ULIDTT
 QGASFL 1 1
 QGASSC 1 1
 QGASTT
 UGASTT
 QEVDFL 1 1
 QEVDFSC 1 1
 QEVPTT
 UEVPTT
 QCNDFL 1 1
 QCNDSC 1 1

QCNDTT
UCNDTT
QOUTTT
UOUTTT
UINTGT
UMCO
FUERR
TOTUO2
END PLOT

6.0 OUTPUT DESCRIPTION

HANSF produces four outputs: a log file, main plot file, MCO-specific file, and tabular output. Each is discussed in detail below.

6.1 Log File

This file produces a record of the HANSF run and its input. The first line of the log file lists the file name of the input deck used for the run. The input file name is followed by the results of fits for gas properties. For each gas in the GASPROP.DAT file, fits for specific heat, second virial coefficient, and viscosity are compared to test values. If the critical temperature for the gas is above 300 K, the fits for critical pressure and heat of vaporization are also listed. A partial example is shown below:

```
Input file AIR.DAT opened for reading
Input file name used for this run is AIR
Properties for 10 Gases read by Amazon
NITROGEN   Cvin: 9.470E+02 Fit: 9.517E+02   Bvin: 1.286E-04 Fit: 1.286E-03
           Mugin: 5.392E-05   Fit: 5.392E-05
OXYGEN     Cvin: 8.810E+02 Fit: 8.826E+02   Bvin: 8.710E-04 Fit: 8.709E-04
           Mugin: 6.399E-05   Fit: 6.399E-05
STEAM      Cvin: 2.653E+03 Fit: 2.195E+03   Bvin: -4.000E-02 Fit: -4.023E-02
           Pcrin: 2.198E+07 Fit: 2.198E+07   Hfgin: 2.438E+06 Fit: 2.440E+06
           Mugin: 1.195E-05   Fit: 1.195E-05
.
.
.
```

The log file shows the number of gases read from GASPROP.DAT and then lists the curve-fit comparisons for all of them. The example here shows only three curve-fit comparisons out of a total of ten, however.

The input file is then echoed, assuming no keywords are misspelled. If a keyword is misspelled, the error is printed to the log file and execution stops. A summary of gas initialization for each region is printed next. These summaries have the following format:


```

Gas initialization for region 1
Gas      Mass Fr  u-form  du(v)  cv,300  du/dt,300
NITROGEN 0.7671 -8.85E+04 -2.07E+02  738.27  738.24
OXYGEN   0.2329 -7.74E+04 -1.96E+02  655.03  655.04

```

Sum of partial pressures/input p = 1.0000

```

Gas initialization for region 2
Gas      Mass Fr  u-form  du(v)  cv,300  du/dt,300
NITROGEN 0.7671 -8.85E+04 -2.07E+02  738.27  738.24
OXYGEN   0.2329 -7.74E+04 -1.96E+02  655.03  655.04

```

Sum of partial pressures/input p = 1.0000

The initialization print-out shows the mass fraction of each gas, integral of the temperature-dependent specific heat (u-form), the contribution to the energy arising from a non-zero virial coefficient (du(v)), the specific heat evaluated at 300 K from the curve fit, and the specific heat evaluated at 300 K based on the derivative of the gas energy with respect to temperature.

At each print interval, a summary of region thermal properties is printed to the log file, as follows:

```

Region properties:                               Time=          0.000 seconds
                                                0.000 hours

Timestep = 0.0100      Average = 0.0100

Region # ->      1      2
Press., Pa      1.013E+05  1.013E+05
Temp., C        5.000E+01  5.000E+01
               , K        3.231E+02  3.231E+02
Spec. Heat Cv   7.208E+02  7.208E+02
Ratio Cp/Cv     1.401E+00  1.401E+00
k, W/m-C        2.758E-02  2.758E-02
rho, kg/m^3     0.109E+01  0.109E+01
mu, Pa-s        0.195E-04  0.195E-04

```

6.2 Plot File

HANSF creates a file with the same name as the input file, but with a PLT extension, that contains a header based on the plot variables specified after the PLOT keyword, and the variable values as a function of time. Consider the following plot variable specification:

```

PLOT      ! Keyword for plotting section
PRESSURE  1      1
GAS-T     5      1  2  3  4  5
HS-TA     5  61  62  63  64  65
HS-TA     6  66  67  68  69  70  71
HS-TI     3  72  73  74
HS-TO     3  72  73  74
HS-TA     6      1  4  7  10  14  15
HS-TA     6  16  19  22  25  29  30
HS-TA     6  31  34  37  40  44  45
HS-TA     6  46  49  52  55  59  60
GAS-X     NITROGEN  5  1  2  3  4  5
GAS-X     OXYGEN    5  1  2  3  4  5
GAS-X     STEAM     5  1  2  3  4  5
GAS-X     HYDROGEN  5  1  2  3  4  5
GAS-X     HELIUM    5  1  2  3  4  5
GAS-W     5  1  2  3  4  5
GAS-WX    5  1  2  3  4  5
GAS-MASS  HYDROGEN  1  7
GAS-MASS  STEAM     1  7
END PLOT  ! PLOT is a comment

```

! Pressure in MCO
! Temperature in MCO
! Scrap 1 + MCO
! Cask, MCO bott & lid
! Cask, MCO bott & lid
! Fuel 2
! Fuel 3
! Fuel 4
! Fuel 1
! N2 %
! O2 %
! H2O %
! H2 %
! He %
! Junc. flow
! Junc. cc flow
! H2 release
! H2O release

This produces the following plot file header and plot values for time zero:

87

```

Amazon Plot
TIME      DELT      ITDX      PR001      TGR001
TGR002    TGR003    TGR004    THSI074    THSO072
TGR005    THSI072    THSI073    THSA014    THSA015
THSO073    THSO074    THSA001    THSA031    THSA034
THSA004    THSA007    THSA010    THSA052    THSA055
THSA016    THSA019    THSA022    THSA065    THSA066
THSA025    THSA029    THSA030    THSA069    WJ003
THSA037    THSA040    THSA044    WJ002      WJ003      WJ004
THSA045    THSA046    THSA049    WJX005    FXNITR01
THSA059    THSA060    THSA061    WJX002    FXHYDR02
THSA062    THSA063    THSA064    WJX005    FXSTEA02    FXHYDR02
THSA067    THSA068    THSA069    WJX005    FXNITR04    FXOXYG04
THSA070    THSA071    WJ001      WJX005    FXHYDR05    FXHELI05
WJ005      WJX001
WJX002    WJX003    WJX004    WJX005    FXNITR01
FXOXYG01  FXSTEA01    FXHYDR01    FXSTEA02    FXHYDR02
FXHELI01  FXNITR02    FXOXYG02    FXSTEA02    FXHYDR02
FXHELI02  FXNITR03    FXOXYG03    FXSTEA02    FXHYDR02
FXSTEA03  FXHYDR03    FXHELI03    FXNITR04    FXOXYG04
FXSTEA04  FXHYDR04    FXHELI04    FXNITR04    FXOXYG04
FXNITR05  FXOXYG05    FXSTEA05    FXHYDR05    FXHELI05
MgSTEA07  MgHYDR07
SEC      SEC
K        K        K
K        K        K
K        K        K
K        K        K
K        K        K
K        K        K
K        K        K
K        K        K

```

K	K	K	K	K	K	K
K	K	K	KG/S	KG/S	KG/S	KG/S
KG/S	KG/S	KG/S	KG/S	KG/S		

kg

kg

0.0000E+00	1.0000E-01	0.0000E+00	1.0130E+05	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02	3.4815E+02
1.2953E-01	1.3703E-01	1.4435E-01	1.5123E-01	1.5172E-01
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7.9000E-01	2.0000E-01	1.0000E-02	0.0000E+00	0.0000E+00
7.9000E-01	2.0000E-01	1.0000E-02	0.0000E+00	0.0000E+00
7.9000E-01	2.0000E-01	1.0000E-02	0.0000E+00	0.0000E+00
7.9000E-01	2.0000E-01	1.0000E-02	0.0000E+00	0.0000E+00
7.9000E-01	2.0000E-01	1.0000E-02	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00			

The first line contains the number of plot variables, which is just the number of variables specified by the PLOT keyword, plus three variables for the time, time step (DELTA), and ITDX. The number of plot variables is useful for plotting packages like LOOK and MULTI-PLOT, which are Fauske and Associates, Inc. products for plotting output files like those produced by HANSF. Note that duplicate plot variables in the PLOT input section are ignored, and a plot variable is counted only once.

ITDX denotes the variable that is limiting the time step, and is useful for debugging and development purposes. ITDX has the following values:

- If the temperature rate-of-change is limiting the time step, ITDX = 100 + IR, where IR is the region number,
- If the pressure rate-of-change is limiting the time step, ITDX = 200 + IR,
- If the aerosol mass rate-of-change is limiting the time step, ITDX = 300 + IR,

- If the heat sink temperature rate-of-change (Side 1) is limiting the time step, $ITDX = 400 + IHS$, where IHS is the heat sink number,
- If the heat sink temperature rate-of-change (Side 2) is limiting the time step, $ITDX = 500 + IHS$, where IHS is the heat sink number, and
- If none of these rates-of-change is limiting the time step, $ITDX = 0$.

Variables names are shown next, followed by units. Values for the variables appear in the same order in which the variable names are listed. Values for time zero are listed here as an example. Of course, new values are listed for simulation times as dictated by the plot interval specified by PLTMIN and PLTMAX.

6.3 Tabular Output File

The tabular output starts with a header that documents the run by listing the code version, time and date of the run, location of the input deck file, and the title from the input deck file.

At the specified print interval, the tabular output file provides a snapshot of conditions in the regions, junctions, heat sinks, fuel basket(s), and scrap basket(s), as well as the current timestep and average timestep over the duration of the run. The snapshot begins with a summary of conditions in the fuel basket(s) and the scrap basket(s), and includes the following:

- heat capacities (J/C) for the cask wall, lid/floor, MCO wall, insert, and scrap basket fin; these appear one time only,
- mass inventories for uranium, oxide, hydride, dehydrided hydride, nitride, free water, sludge, hydrated sludge, water in sludge, free water on insert, and free water on MCO wall; these appear for each fuel basket, each scrap basket, and the entire MCO,
- heat capacity of fuel/scrap, including water on fuel/scrap,

- fuel exposed area, fuel oxidation area, hydride oxidation area, and MCO wall area available for heat transfer; these appear for each fuel basket, each scrap basket, and the entire MCO,
- heat sources, namely decay heat, oxidation, nitriding, and hydriding; these appear for each fuel basket, each scrap basket, and the entire MCO,
- heat losses, namely radiation/convection to the MCO wall, radiation to lid/floor, convection to MCO gas, evaporation/dehydration/radiolysis, and conduction to other heat sinks; these appear for each fuel basket, each scrap basket, and the entire MCO,
- for each fuel and scrap basket, temperatures are printed out along with corresponding insert and MCO wall temperatures; only inner elements are considered,
- total internal energy in the entire MCO, which includes fuel, scrap and water on fuel/scrap, as calculated from a snapshot of mass, temperature, and specific heat,
- integrated energy which is equal to (initial total internal energy + integrated sources - integrated losses) for the entire MCO, and
- relative error between total internal energy and integrated energy; this is essentially a check on the HANSF energy balance.

The following region variables are printed out:

- Temperature,
- Pressure,
- Thermal Properties: specific heat at constant volume, ratio of specific heats, density, thermal conductivity, and dynamic viscosity,
- Mole Fractions of Gas,
- Gas Masses,
- Relative Humidities,
- Aerosol Masses,
- Liquid Masses, and
- Rates-of-Change of Gas and Aerosol.

The following junctions variables are printed out for each junction:

- Temperature ($^{\circ}\text{C}$) of each node, and
- Boundary Conditions on each side.

At the end of the output, the peak temperatures and pressures in each region and the time they occurred are printed. Also, the peak hydrogen generation rate in the MCO and the corresponding time is printed.

```
Time & Date of Run:      16:36:13.87      12/08/98
Input Deck: C:\HANSF13\VALIDATION\HSPRIN\HSPRINT.DAT  58,147  12-08-98  4:36
STEADY STATE WITH DECAY HEAT
```

cask wall	7.165E+06
lid/floor	3.886E+05
MCO wall	2.794E+05
insert	0.000E+00
scrap bskt fin	2.883E+04

	fuel basket 1	fuel basket 2	fuel basket 3
uranium mass (kg)	1357.127	1357.127	1357.127
oxide mass (kg)	0.000	0.000	0.000
hydride mass (kg)	0.142	0.142	0.142
dehydrodized hydride mass (kg)	0.000	0.000	0.000

nitride mass (kg)	0.000	0.000	0.000
water on fuel (kg)	0.101	5.999	0.000
sludge mass (kg)	5.200	5.200	5.200
hydrated sludge mass (kg)	0.901	0.901	0.901
water in sludge (kg)	0.101	0.101	0.101
heat capacity of fuel (J/C)	176426.	176426.	176426.
water on insert (kg)	0.000	0.000	0.000
water on MCO (kg)	0.000	0.000	0.000
fuel exposed area (m ²)	0.875	0.875	0.875
fuel oxidation area (m ²)	8.752	8.752	8.752
hydride oxidation area (m ²)	10.502	10.502	10.502
MCO wall area (m ²)	1.100	1.100	1.100
decay power (W)	155.297	155.297	155.297
oxidation power (W)	0.000	0.000	0.000
nitriding power (W)	0.000	0.000	0.000
hydriding power (W)	0.000	0.000	0.000
rad/conv loss to MCO wall(W)	0.000	0.000	0.000
rad loss to lid/floor (W)	0.000	0.000	0.000
conv loss to gas (W)	0.000	0.000	0.000
evap/dehyd/radioly loss (W)	0.000	0.000	0.000
cond loss to other hs (W)	0.000	0.000	0.000
	fuel basket 4	scrap basket 1	MCO total
uranium mass (kg)	1357.127	980.742	6409.249
oxide mass (kg)	0.000	0.000	0.000
hydride mass (kg)	0.142	0.730	1.297
dehydrated hydride mass (kg)	0.000	0.000	0.000
nitride mass (kg)	0.000	0.000	0.000
water on fuel (kg)	0.000	0.000	6.099
sludge mass (kg)	0.000	0.000	15.600
hydrated sludge mass (kg)	0.000	0.000	2.702
water in sludge (kg)	0.000	0.000	0.302
heat capacity of fuel (J/C)	176426.	127496.	833202.
water on insert (kg)	0.000	0.000	0.000
water on MCO (kg)	0.000	0.000	0.000
fuel exposed area (m ²)	0.875	4.503	8.004
fuel oxidation area (m ²)	8.752	45.032	80.039
hydride oxidation area (m ²)	10.502	54.039	96.047
MCO wall area (m ²)	1.100	1.100	5.500
decay power (W)	155.297	112.227	733.417
oxidation power (W)	0.000	0.000	0.000
nitriding power (W)	0.000	0.000	0.000
hydriding power (W)	0.000	0.000	0.000
rad/conv loss to MCO wall(W)	0.000	0.000	0.000
rad loss to lid/floor (W)	0.000	0.000	0.000
conv loss to gas (W)	0.000	0.000	0.000
evap/dehyd/radioly loss (W)	0.000	0.000	0.000
cond loss to other hs (W)	0.000	0.000	0.000
MCO scrap/fuel temp.(only inner elements):	Time=		0.000 seconds
	insert	fuel/scrap	0.000 hours
			MCO wall
scrap- 1	50.0 50.0 50.0 50.0 50.0 50.0 50.0 50.0 50.0		50.0

fuel- 1	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
fuel- 2	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
fuel- 3	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
fuel- 4	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0

total energy in fuel 2.77488E+08 J
integrated energy 2.77488E+08 J
relative error 0.00000E+00

Region properties: Time= 0.000 seconds
0.000 hours

Timestep = 0.1000 Average = 0.1000

Region # ->	1	2	3	4	5
Press., Pa	1.013E+05	1.013E+05	1.013E+05	1.013E+05	1.013E+05
Temp., C	5.000E+01	5.000E+01	5.000E+01	5.000E+01	5.000E+01
, K	3.231E+02	3.231E+02	3.231E+02	3.231E+02	3.231E+02
Spec. Heat Cv	3.515E+03	3.515E+03	3.515E+03	3.515E+03	3.515E+03
Ratio Cp/Cv	1.426E+00	1.426E+00	1.426E+00	1.426E+00	1.426E+00
k, W/m-C	1.267E-01	1.267E-01	1.267E-01	1.267E-01	1.267E-01
rho, kg/m^3	2.090E-01	2.090E-01	2.090E-01	2.090E-01	2.090E-01
mu, Pa-s	1.810E-05	1.810E-05	1.810E-05	1.810E-05	1.810E-05

Mole fractions of gas ...					
STEAM	1.100E-01	1.100E-01	1.100E-01	1.100E-01	1.100E-01
HELIUM	8.900E-01	8.900E-01	8.900E-01	8.900E-01	8.900E-01

Gas masses ...					
STEAM	7.468E-03	7.468E-03	7.468E-03	7.468E-03	7.468E-03
HELIUM	1.343E-02	1.343E-02	1.343E-02	1.343E-02	1.343E-02

Relative humidities ...					
STEAM	8.975E+01	8.975E+01	8.975E+01	8.975E+01	8.975E+01

Aerosol masses ...

Liquid masses ...

Rates of change of gas and aerosol ...

Region # ->	6	7
Press., Pa	1.013E+05	1.013E+05
Temp., C	5.000E+01	5.000E+01
, K	3.231E+02	3.231E+02
Spec. Heat Cv	4.180E+03	7.208E+02
Ratio Cp/Cv	1.000E+00	1.401E+00
k, W/m-C	6.493E-01	2.758E-02
rho, kg/m^3	1.169E+03	1.088E+00
mu, Pa-s	5.471E-04	1.947E-05

Mole fractions of gas ...		
NITROGEN	0.000E+00	7.900E-01
OXYGEN	0.000E+00	2.100E-01
WATER	1.000E+00	0.000E+00

Gas masses ...		
NITROGEN	0.000E+00	8.345E+08
OXYGEN	0.000E+00	2.534E+08
WATER	2.922E+02	0.000E+00

Relative humidities ...		
WATER	3.535E+01	0.000E+00

Aerosol masses ...

Liquid masses ...

Rates of change of gas and aerosol ...

Junction Flowrates:

Time= 0.000 seconds
0.000 hours

Path # ->	1	2	3	4	5
W: kg/s	-3.928E-06	-5.901E-06	-5.919E-06	-3.922E-06	0.000E+00
Wcc: kg/s	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Heat sink temperatures:

Time= 0.000 seconds
0.000 hours

HS # 1	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 2	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 3	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 4	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 5	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 6	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 7	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 8	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS # 9	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					
HS #10	(insulated)	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000	50.000	50.000	50.000	50.000	50.000
	50.000 (insulated)					

6.4 Restart File

HANSF writes a restart file with the same file name as the input file, but with a REW extension. This file can be used for subsequent restart runs. At the interval specified by the input file, HANSF writes the conditions and rates-of-change needed to restart the run. Restart files are not scrutable and an example is not included here.

6.5 MCO-Specific Plot File

HANSF creates an MCO-specific plot file, with an extension PL1, much like the main plot file described in Section 6.2. Consider the following input for the PLOT sub-section of the MCO section:

```

PLOT
QDECTT      ! TOTAL DECAY HEAT
QOXOTT      ! OXIDATION - OXYGEN
QOXWTT      ! OXIDATION - STEAM
QHYDTT      ! HYDRIDING POWER
QINTT       ! TOTAL SOURCES
QMCOTT      ! LOSSES TO MCO
QLIDTT      ! LOSSES TO LID AND BOTTOM
QGASTT      ! LOSSES TO GAS
QEVPTT      ! LOSSES TO EVAPORATION
QOUTTT      ! TOTAL LOSSES
END

```

In the example that follows, the first line lists the number of plot variables, followed by lines for the variable names and units, for the input above. The values at time zero are then shown. Of course, the PL1 file contains values for the entire simulation time as dictated by min/max plotting interval, etc.

11

```

Amazon Plot
TIME      QDECTT      QOXOTT      QOXWTT      QHYDTT      QINTT
QMCOTT    QLIDTT
QGASTT    QEVPTT      QOUTTT
SEC       W          W          W          W          W
W         W          W

```

0.0000E+00	7.3342E+02	0.0000E+00	1.3701E+02	8.3999E-03
8.7043E+02	-6.7635E-08	-1.0487E-05	8.5553E-02	9.0227E+03
9.0228E+03				

7.0 SEPARATE EFFECTS TESTING

Separate effects tests are conducted to validate the correct function of models for individual phenomena. Separate effects tests are described here for the following phenomena: (1) region thermodynamics, (2) fog formation, (3) inter-compartmental flow, (4) heat transfer modeling, (5) aerosol transport and deposition, (6) counter-current flow, (7) aerosol de-entrainment, (8) evaporation, (9) hydride formation and decomposition, (10) uranium oxidation, (11) entrainment, (12) hydrate decomposition, (13) fuel and scrap basket heat transfer, (14) nitriding, (15) vacuum and recirculation pump, (16) radiation networks, and (17) overall energy balance. Input files for these tests appear in Appendix A.

7.1 Region Thermodynamics

Essential thermodynamic model features requiring validation are:

1. Constitutive Relations. An increment in system internal energy should yield the correct increment in pressure and temperature (discussed here).
2. Aerosol Equilibrium. An initially non-equilibrium state requiring formation or depletion of aerosols should evolve to the correct equilibrium state (see Section 7.2).
3. Dynamic Evolution. A system with mass inflows and outflows should have the correct pressure and temperature history, illustrating correct conservation laws and property calculations (see Section 7.3).

Constitutive relations are validated for the non-ideal gas steam by using steam table data. A reference state is defined, and states with the same specific volume at higher energies are identified as shown in Table 7-1. By initializing a region to the reference state and then adding an energy source, the higher energy states should be duplicated. The precision of this procedure depends upon the integral agreement between the curve fits for $c_v(T)$ and $B(T)$ with the steam table values [Keenan, et al, 1978]. Very good agreement is shown in Table 7-1 over a large

Table 7-1: <u>Constitutive Relation Validation</u>				
A. <u>Steam Table State</u> [Keenan, et al, 1978]				
v (m ³ /kg)	P (MPa)	T (°C)	u (kJ/kg)	Δu (kJ/kg)
0.4011	0.46	145	2551.8	0
0.4010	0.72	360	2895.6	343.8
0.4011	1.00	600	3296.8	745.0
0.4034	1.80	1300	4679.5	2127.7
B. <u>Calculated State</u>				
ΔU = Δu/v (kJ)	P (MPa)	T (°C)		
0.0	0.46	145		
857.4	0.723	364		
1857.9	1.005	606		
5306.0	1.819	1309		

temperature range from an initially supersaturated state to a high super-heated state. It is also notable that the non-ideal gas contribution to the internal energy is about 20% of the ideal contribution for the initial condition, so the model must be correct in order for agreement to be achieved.

7.2 Fog Formation

The fog (aerosol) formation model is checked by a sample problem with an initially supersaturated vapor (relative humidity greater than 100%). When fog forms, the gas temperature increases and at equilibrium the relative humidity is 100%. The temperature rise and aerosol mass are given by:

$$\Delta T = \frac{m_{io} (RH - 1) / RH}{\frac{C_o}{u_{fg}} + \frac{m_{io} \theta}{RH}} \quad (7-1)$$

$$m_{ai} = \frac{C_o}{u_{fg}} \Delta T \quad (7-2)$$

$$\theta = \frac{1}{P_{sat}} \frac{dP_{sat}}{dT} - \frac{1}{T} \quad (7-3)$$

where m_{io} = Initial vapor mass, kg,
 RH = Relative humidity,
 C_o = Gas heat capacity, J/K,
 u_{fg} = Energy change of vaporization, J/kg,
 T = Temperature, K, and
 P_{sat} = Saturation pressure, Pa.

Table 7-2 contains the sample problem initial conditions, analytical solution, and output of the calculation, illustrating very good agreement. The reason for a few percent error is that the derivative dP_{sat}/dT varies over the range of ΔT so that the linear analytical extrapolation is imperfect.

7.3 Inter-Compartmental Flow

An integral check of the junction flow model, conservation of mass and energy, and correct property calculations for flow between compartments is prediction of the pressure history for a region with a fixed inlet source rate and a fixed outlet downstream pressure. Rates-of-change of mass, temperature, and pressure for an ideal gas in an adiabatic region with these flows are:

$$\frac{dm}{dt} = W_s - W_o \quad (7-4)$$

$$\frac{dT}{dt} = \left(\frac{W_s}{m} \right) (\gamma T_s - T) + \left(\frac{W_o}{m} \right) (\gamma - 1) T \quad (7-5)$$

$$\frac{dP}{dt} = \left(\frac{\gamma RT}{MV} \right) \left(W_s \frac{T_s}{T} - W_o \right) \quad (7-6)$$

Table 7-2: Fog Formation Sample Problem

A. <u>Initial Quantities</u>			
Temperature	T_o	323	K
Saturation Pressure	P_{sat}	12350	Pa
Pressure Derivative	dP_{sat} / dT	636	Pa/K
Internal Energy Change	u_{fg}	2.23	MJ/kg
Steam Mole Fraction		0.15	
Nitrogen Mole Fraction		0.85	
Steam Specific Heat		1409.	J/kgK
Nitrogen Specific Heat		739.	J/kgK
Steam Mass	m_{io}	0.1006	kg
Relative Humidity	RH_{io}	1.2	
Nitrogen Mass		0.8871	kg
Gas Heat Capacity	C_o	798	J/K
B. <u>Analytical Solution</u>			
Parameter	θ	4.840E-2	
Temperature Rise		3.80	K
Aerosol Mass		1.36E-3	kg
C. <u>Code Output</u>			
Temperature Rise		3.82	K
Aerosol Mass		1.373E-3	kg

where W_s and T_s are the constant source flowrate and temperature, W_o is the outlet flowrate found from the compressible flow relation, and the ideal gas of molecular weight M and specific heat ratio γ applies to the source and the region initial conditions. The preceding simple equations are easily solved numerically (pressure dependence of W_o makes analytic solution impossible) and are verifiable because the pressure equation is redundant (the ideal gas law provides P given m and T).

A test case is defined in Table 7-3 illustrating an "overdriven" source wherein a maximum in pressure is obtained because the outflow rate depends upon both gas density and pressure. Figure 7-1 shows the pressure history and achievement of a steady-state with equal region and source temperatures and a pressure high enough to equate source and vent flows. Model results are identical to the simplified equations. From the test case data, the ideal gas law, and final pressure, the final region density is 0.1886 kg/m^3 , the pressure ratio is 0.893, and

Figure 7-1: Pressure History for Ideal Gas Source and Outflow Test Case.

- HANSF and Simple Model Results are Identical.

Table 7-3: Test Case Values

Volume	850	m ³
Pressure	10 ⁵	Pa
Temperature	300	K
Specific heat	830	J/kg·K
Molecular weight	28	kg/kg·mole
Sink Pressure	10 ⁵	Pa
Vent area	0.03	m ²
Vent coefficient	0.5345	(1 / $\sqrt{3.5}$)
Source rate	1.0	kg/s
Source temperature	2000	K

7.4 Heat Sink Modeling

The model for heat transfer to passive heat sinks can be validated using the problem of a one-dimensional slab exposed at time zero to a fluid at constant temperature T_{∞} on one surface, and insulated on the other. The slab has thickness L , uniform initial temperature T_i , thermal conductivity k , specific heat c , and density ρ . Consider the following values for the validation problem:

$$\begin{aligned}
 L &= 10 \text{ cm,} \\
 T_{\infty} &= 100^{\circ}\text{C,} \\
 T_i &= 200^{\circ}\text{C,} \\
 k &= 0.5 \text{ W/m}\cdot\text{K,} \\
 c &= 500 \text{ J/kg}\cdot\text{K,} \\
 \rho &= 5000 \text{ kg/m}^3, \text{ and,} \\
 \alpha &= 2 \times 10^{-7} \text{ m}^2/\text{s.}
 \end{aligned}$$

Simulation of this problem uses a single region with one plane wall heat sink. Models for junction flow, aerosol settling, etc., are neglected. The region volume is made extremely large ($1 \times 10^{10} \text{ m}^3$) to keep the temperature constant regardless of any heat transfer to/from the heat sink. Initial gas temperature is 100°C , initial pressure is $100,000 \text{ Pa}$, and the region is 80% oxygen, 20% nitrogen by volume. The heat sink has the dimensions and thermal properties noted above, with no volumetric heat generation. Characteristic height, which is used to determine the natural convection heat transfer coefficient, is 10 m , and the heat sink one-sided surface area is 100 m^2 . Wall emissivity equals 0.7 .

The approach here is to compare model results against approximate analytical solutions using a constant heat transfer coefficient. Initially, the slab temperature profile can be approximated by the solution for a semi-infinite slab exposed at time zero to a fluid with constant h [Incropera and DeWitt, 1981]:

$$\frac{T(x, t) - T_i}{T_\infty - T_i} = \operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right) - \left[\exp\left(\frac{hx}{k} + \frac{h^2 \alpha t}{k^2}\right)\right] \left[\operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}} + \frac{h\sqrt{\alpha t}}{k}\right)\right] \quad (7-7)$$

Equation (7-7) applies if the transient time is much less than the time constant for conduction (L^2 / α), which is $50,000$ seconds. The heat transfer coefficient h is evaluated using equations (2-11) through (2-15), assuming $T_\infty = 150^\circ\text{C}$ (average of 100°C and 200°C), $T_i = 200^\circ\text{C}$, and the thermal properties of the gas are the thermal properties of air at 400 K . The natural convection heat transfer coefficient is $4 \text{ W/m}^2\text{-K}$, and the radiative natural convection is $7 \text{ W/m}^2\text{-K}$, for a total of $11 \text{ W/m}^2\text{-K}$. For the first $50,000$ seconds of the transient, Table 7-4 compares the surface temperature as predicted by equation (7-7) against HANSF results. For the first $50,000$ seconds, the two sets of results are in good agreement. Afterwards, the slab is no longer semi-infinite and the heat transfer coefficient is no longer $11 \text{ W/m}^2\text{-K}$.

If the heat sink no longer behaves as if it were semi-infinite, Heisler charts can be used to estimate the temperature at the adiabatic surface and the temperature distribution in the heat sink. For the problem statement, Heisler charts give a non-dimensional solution assuming h is

Table 7-4:
Comparison of the Semi-Infinite Slab Solution for
Surface Temperature (T_o) with Model Results

Time (seconds)	Model (°C)	Analytical (°C)
0	200.000	200.000
1000	172.715	170.75
2000	164.795	163.05
3000	159.645	158.25
4000	155.817	154.75
5000	152.779	151.95
10000	143.220	143.45
20000	134.046	134.25
30000	129.125	127.65
40000	125.902	122.55
50000	123.572	118.35

constant [Incropera and DeWitt, 1981]. Non-dimensional temperature at the adiabatic surface, θ_L , is defined by:

$$\theta_L = \frac{T_L - T_\infty}{T_i - T_\infty} \quad (7-8)$$

where T_L is the temperature at the adiabatic surface. Values for θ_L are plotted as a function of the Fourier number ($\alpha t/L^2$) and the inverse Biot number (k/hL). Temperature distribution through the slab is expressed non-dimensionally as

$$\theta = \frac{T - T_\infty}{T_L - T_\infty} \quad (7-9)$$

Heisler charts express θ as a function of the inverse Biot number and the non-dimensional coordinate, x/L . Initially, the inverse Biot number is 0.45, but it increases over the course of

the transient as the natural convection and radiation heat transfer coefficients decrease. Table 7-5 shows a comparison of model results with analytical results using the Heisler charts. Results are in good agreement, although the comparison is limited by the ability to read the charts and the assumption of constant heat transfer coefficient. Nevertheless, Tables 7-4 and 7-5 validate the model heat transfer model.

**Table 7-5: Comparison of Model Results With Analytical Results
Obtained from Heisler Charts**

Time (seconds)	Model Results T_o ($^{\circ}\text{C}$)	Model Results T_L ($^{\circ}\text{C}$)	F_o	Bi^{-1}	Analytical Results T_o ($^{\circ}\text{C}$)	Analytical Results T_L ($^{\circ}\text{C}$)
50,000	136.65	118.35	1	0.45	135	115.8
100,000	112.75	106.85	2	0.45	110	104.5
150,000	104.75	102.65	3	0.45	103	101.4
200,000	101.85	101.05	4	0.45	100.9	100.4
250,000	100.75	100.45	5	0.45	100.3	100.1

7.5 Aerosol Transport and Deposition

7.5.1 Sedimentation

Implementation of the aerosol modeling is validated by comparison to the well-known AB-5 experiment conducted at Hanford [Hilliard, et al, 1983]. In this experiment, a sodium vapor source reacted to produce sodium oxide aerosol during a source period of 900 s into a volume of 850 m³ at a rate of 0.444 kg/s.

Figure 7-2 illustrates the suspended mass versus time as both measured and using the present code and correlation technique. Results are considered very good - within a factor of two for a suspended mass history spanning four orders of magnitude.

Figure 7-2: Suspended Mass History for AB-5 Data (boxes) and Prediction (line).

7.5.2 Leakage

Consider two regions of pure nitrogen connected by a single junction. If the first region initially has a higher pressure than the second, a mass flowrate results and continues until the pressure differential between the two volumes is zero. If the first volume contains an aerosol concentration initially and the second volume does not, aerosol leaks from the first volume to the second until the two pressures equilibrate.

Assume the first region has an initial pressure of 0.12 MPa, an initial temperature of 300 K, and an initial CsOH aerosol concentration of 0.001. Its volume is made $1 \times 10^4 \text{ m}^3$ to keep pressure, temperature, and aerosol concentration constant. The second region has an initial pressure of 0.10 MPa, an initial temperature of 300 K, and no initial CsOH aerosol mass. Its volume is 1 m^3 . The only aerosol transport mechanism is leakage from the first volume to the second.

After the flow equilibrates, the mass lost from the first region is equal to the mass gained by the second region. The aerosol mass that leaks into the second region is given by:

$$\Delta M_{\text{Cs}} = \frac{\Delta M_{\text{N}_2}}{\rho_1} C_1 \quad (7-10)$$

where ΔM_{Cs} is the mass of cesium hydroxide aerosol in the second region, ΔM_{N_2} is the mass of nitrogen lost from the first region (or gained by the second region), ρ_1 is the density of nitrogen in the first region, and C_1 is the CsOH aerosol concentration in the first region. The density of nitrogen in the first region is obtained by the ideal gas law:

$$\rho_1 = \frac{0.12 \times 10^6 \text{ Pa}}{\left(\frac{8314}{28} \frac{\text{m}^2}{\text{s}^2 \cdot \text{K}} \right) (300 \text{ K})} = 1.3471 \frac{\text{kg}}{\text{m}^3} \quad (7-11)$$

The nitrogen mass gained by the second region is obtained by comparing the initial nitrogen mass to the equilibrium mass.

$$\Delta M_{N_2} = 1.283 \text{ kg} - 1.123 \text{ kg} = 0.160 \text{ kg} \quad (7-12)$$

The mass of CsOH aerosol that enters the second region is then:

$$\Delta M_{Cs} = \frac{(0.16 \text{ kg}) (0.001 \text{ kg/m}^3)}{1.3471 \text{ kg/m}^3} = 1.188 \times 10^{-4} \text{ kg} \quad (7-13)$$

This is in excellent agreement with the value of $1.188 \times 10^{-4} \text{ kg}$, as shown in Figure 7-3.

7.6 Counter-Current Flow

To validate the counter-current flow model in the HANSF code, a sample problem was devised and code calculation results were compared with hand-calculations. Two compartments, each with volume of 100 m^3 , were arranged one on top of the other. They were connected by a horizontal junction (junction in a horizontal wall) with dimensions of $1.9 \text{ m} \times 2.1 \text{ m} \times 0.5 \text{ m}$. Initially, the lower compartment contains warmer air than the upper compartment (333.15 K vs. 293.15 K).

Figure 7-4 shows counter-current flow rate through the junction. There is no uni-directional flow because two compartments are initialized with equal pressure. However, because a heavier gas sits above, a strong counter-current flow develops in the junction. The magnitude of the counter-current flow diminishes as the two compartments approach equilibrium, as shown in Figure 7-5.

Calculation of pure counter-current flow through a rectangular junction in a horizontal wall is based on the following correlation [Epstein, 1988]:

$$\frac{Q_{cc}}{(D^5 g \Delta \rho / \bar{\rho})^{1/2}} = \frac{0.055 \left[1 + 400 \left(\frac{L}{D} \right)^3 \right]^{1/6}}{\left\{ 1 + 0.00527 \left[1 + 400 \left(\frac{L}{D} \right)^3 \right]^{1/2} \left[\left(\frac{L}{D} \right)^6 + 117 \left(\frac{L}{D} \right)^{3/4} \right]^{1/3} \right\}} \quad (7-14)$$

Figure 7-3: Output for Aerosol Leakage Validation.

```

region properties at time      3.500 seconds
Timestep =      .0100   Average =      .0100

Region # ->          1              2
Temperature K        300.00        315.07
Pressure Pa    1.19998E+05    1.19993E+05

Mole fractions of gas ...
NITROGEN          1.000E+00        1.000E+00

Gas masses ...
NITROGEN          1.348E+04        1.283E+00

Relative humidities ...

Aerosol masses ...
CSOH              1.000E+01        1.188E-04

Liquid masses ...

Rates of change of gas and aerosol ...

Spec. heat Cv by region:
    7.375E+02    7.388E+02

Ratio Cp/Cv by region:
    1.403E+00    1.403E+00

Flowrates at time      3.500

Path # -> 1
W: kg/s    -8.861E-05
Wcc: kg/s   0.000E+00

```


Figure 7-4: Counter-Current Flow Rate Through Junction.

Figure 7-5: Compartment Temperatures for Counter-Current Flow Validation.

- where Q_{cc} = purely buoyancy-driven exchange volumetric flow rate,
 D = hydraulic diameter,
 L = length of the junction,
 g = gravitational acceleration (9.81 m/sec^2),
 $\Delta\rho$ = density difference, and
 $\bar{\rho}$ = mean density.

For the junction in this sample case,

$$\begin{aligned}
 D &= 1.1 (W^2 H^3)^{1/5} \\
 &= 1.1 [(1.9\text{m})^2 (2.1 \text{ m})^3]^{1/5} \\
 &= 2.22 \text{ m}
 \end{aligned}
 \tag{7-15a}$$

and

$$L = 0.5 \text{ m} \tag{7-15b}$$

Hence, the Froude number in equation (7-14) becomes 0.07212. That is,

$$\frac{Q_{cc}}{(D^5 g \Delta\rho / \bar{\rho})^{1/2}} = 0.07212 \tag{7-16}$$

At 200 seconds, the air densities in the two compartments were 1.1070 kg/m^3 and 1.1366 kg/m^3 . Therefore, the exchange volumetric flow is given by

$$\begin{aligned}
 Q_{cc} &= 0.07212 (D^5 g \Delta\rho / \bar{\rho})^{1/2} \\
 &= 0.07212 \left[(2.22 \text{ m})^5 (9.81 \text{ m/sec}^2) \left(\frac{0.0296}{1.1218} \right) \right]^{1/2} \\
 &= 0.269 \text{ m}^3/\text{sec}
 \end{aligned}
 \tag{7-17}$$

The equivalent mass flow rate is given by

$$\begin{aligned}
 W_{cc} &= \bar{\rho} Q_{cc} \\
 &= (1.1218 \text{ kg/m}^3) (0.269 \text{ m}^3/\text{sec}) \\
 &= 0.302 \text{ kg/sec}
 \end{aligned}
 \tag{7-18}$$

This is consistent with the code calculated value of 0.303 kg/sec.

Next, mass and energy balance during the exchange flow process was verified. At the beginning, there were 92.00 kg of nitrogen, 26.61 kg of oxygen, and 0.7483 kg of steam in the upper compartment and 80.94 kg of nitrogen, 23.41 kg of oxygen, and 0.6583 kg of steam in the lower compartment. At 200 seconds, there were 87.62 kg of nitrogen, 25.34 kg of oxygen, and 0.7126 kg of steam in the upper compartment and 85.32 kg of nitrogen, 24.67 kg of oxygen, and 0.6940 kg of steam in the lower compartment. Hence, the total mass of each gas species is conserved (i.e., 172.9 kg of nitrogen, 50.02 kg of oxygen, and 1.407 kg of steam).

Initially, the upper compartment was at 293.15 K and the lower compartment was at 333.15 K. At 200 seconds, the upper compartment was at 307.8 K. The specific heat of the gas was 721.4 J/kg-°C for the upper compartment and 727.4 J/kg-°C for the lower compartment. Then, the expected temperature of the lower compartment at 200 seconds to conserve the energy is given by solving

$$\begin{aligned}
 & (119.4 \text{ kg}) (721.4 \text{ J/kg-}^\circ\text{C}) (307.8 \text{ K} - 293.15 \text{ K}) \\
 & + (105.0 \text{ kg}) (727.4 \text{ J/kg-}^\circ\text{C}) (T_2 - 333.15 \text{ K}) \\
 & = 0
 \end{aligned}
 \tag{7-19a}$$

or

$$T_2 = 316.6 \text{ K} \tag{7-19b}$$

The hand-calculated lower compartment temperature at 200 seconds agrees with the code result of 316.2 K.

7.7 De-Entrainment

The aerosol de-entrainment model was validated by considering two compartments connected by a single junction with one 90° bend. At time zero, one compartment has a higher pressure than the other, which causes a mass flow rate that continues until the two compartments equilibrate. The first volume has aerosols whereas the second compartment does not.

Consequently, the aerosol will be transported to the second compartment with some de-entrained in the single 90° bend in the junction; the de-entrained aerosol becomes the liquid aerosol mass in the second compartment.

The first region has an initial pressure of 0.12 MPa, an initial temperature of 300 K, and the initial CsOH aerosol concentration of 0.001. The second region has an initial pressure of 0.10 MPa, an initial temperature of 300 K and has no CsOH aerosol concentration. (These are essentially the same conditions as those used for the aerosol leakage validation in Section 7.5.) The junction between the two compartments was specified to have one 90° bend. Only the aerosol transport and aerosol de-entrainment in the 90° bend models are used.

The test simulation lasts only 0.25 seconds - the time it took to equilibrate the compartment pressures. At the end of 0.001 seconds, 80.1% of the transported CsOH aerosols had been de-entrained in the 90° bend and at the end of the run, a total of 74.2% of the aerosol transported had been de-entrained as shown in Figure 7-6. For comparison the same case run without any bend in the junction, all the aerosol remained in the gas space as shown in Figure 7-7. The total CsOH mass (1.0821×10^{-4}) transported was the same for both cases. Because the de-entrainment efficiency is a function of particle distribution, size, and mass, the efficiency was checked manually at 0.001 seconds. Equation (2-34) was evaluated for each of the 30 aerosol size bins that HANSF uses, based on HANSF output for the particle diameter and mass fraction for each bin. The total de-entrainment efficiency is calculated to be 80.1%, which is in excellent agreement with the results in Figure 7-6.

7.8 Evaporation/Condensation Validation

The evaporation/condensation model was validated using the following test conditions:

- A single-volume MCO with one fuel basket,
- Isothermal conditions (fuel, gas, and heat sinks) at 50°C,

Figure 7-6: Aerosol De-Entrainment Model Validation Test (With 90° Bend).

Region properties:

Time=

0.001 seconds
0.000 hours

Timestep = 0.0010 Average = 0.0010

Region # ->	1	2
Press., Pa	1.200E+05	1.001E+05
Temp., C	2.684E+01	2.697E+01
, K	3.000E+02	3.001E+02
Spec. Heat Cv	7.375E+02	7.375E+02
Ratio Cp/Cv	1.404E+00	1.404E+00
k, W/m-C	2.600E-02	2.601E-02
rho, kg/m^3	0.135E+01	0.112E+01
mu, Pa-s	0.178E-04	0.178E-04

Mole fractions of gas ...

NITROGEN	1.000E+00	1.000E+00
----------	-----------	-----------

Gas masses ...

NITROGEN	1.348E+01	1.124E+00
----------	-----------	-----------

Aerosol masses ...

CSOH	9.999E-03	1.605E-07
------	-----------	-----------

Liquid masses ...

CSOH	0.000E+00	6.712E-07
------	-----------	-----------

Rates of change of gas and aerosol ...

CSOH	a	-8.290E-04	1.603E-04
------	---	------------	-----------

Junction Flowrates:

Time=

0.001 seconds
0.000 hours

Path # ->	1
W: kg/s	1.118E+00
Wcc: kg/s	0.000E+00

Region properties:

Time=

0.249 seconds
0.000 hours

Timestep = 0.0010 Average = 0.0010

Region # ->	1	2
Press., Pa	1.182E+05	1.182E+05
Temp., C	2.554E+01	4.063E+01
, K	2.987E+02	3.138E+02
Spec. Heat Cv	7.374E+02	7.387E+02
Ratio Cp/Cv	1.404E+00	1.404E+00
k, W/m-C	2.592E-02	2.687E-02
rho, kg/m^3	0.133E+01	0.127E+01
mu, Pa-s	0.178E-04	0.185E-04

Mole fractions of gas ...

NITROGEN	1.000E+00	1.000E+00
----------	-----------	-----------

Gas masses ...

NITROGEN	1.334E+01	1.269E+00
----------	-----------	-----------

Aerosol masses ...

CSOH	9.892E-03	2.789E-05
------	-----------	-----------

Liquid masses ...

CSOH	0.000E+00	8.026E-05
------	-----------	-----------

Rates of change of gas and aerosol ...

CSOH	a	-2.095E-07	2.071E-07
------	---	------------	-----------

Junction Flowrates:

Time=

0.249 seconds
0.000 hours

Path # ->	1
W: kg/s	2.824E-04
Wcc: kg/s	0.000E+00

Figure 7-7: Aerosol De-Entrainment Model Validation Test (Without Bend).

Region properties: Time= 0.001 seconds
0.000 hours

Timestep = 0.0010 Average = 0.0010

Region # ->	1	2
Press., Pa	1.200E+05	1.001E+05
Temp., C	2.684E+01	2.697E+01
, K	3.000E+02	3.001E+02
Spec. Heat Cv	7.375E+02	7.375E+02
Ratio Cp/Cv	1.404E+00	1.404E+00
k, W/m-C	2.600E-02	2.601E-02
rho, kg/m^3	0.135E+01	0.112E+01
mu, Pa-s	0.178E-04	0.178E-04

Mole fractions of gas ...
NITROGEN 1.000E+00 1.000E+00

Gas masses ...
NITROGEN 1.348E+01 1.124E+00

Aerosol masses ...
CSOH 9.999E-03 8.316E-07

Junction Flowrates: Time= 0.001 seconds
0.000 hours

Path # -> 1
W: kg/s 1.118E+00
Wcc: kg/s 0.000E+00

Region properties: Time= 0.249 seconds
0.000 hours

Timestep = 0.0010 Average = 0.0010

Region # ->	1	2
Press., Pa	1.182E+05	1.182E+05
Temp., C	2.554E+01	4.063E+01
, K	2.987E+02	3.138E+02
Spec. Heat Cv	7.374E+02	7.387E+02
Ratio Cp/Cv	1.404E+00	1.404E+00
k, W/m-C	2.592E-02	2.687E-02
rho, kg/m^3	0.133E+01	0.127E+01
mu, Pa-s	0.178E-04	0.185E-04

Mole fractions of gas ...
NITROGEN 1.000E+00 1.000E+00

Gas masses ...
NITROGEN 1.334E+01 1.269E+00

Aerosol masses ...
CSOH 9.892E-03 1.082E-04

Junction Flowrates: Time= 0.249 seconds
0.000 hours

Path # -> 1
W: kg/s -6.677E-04
Wcc: kg/s 0.000E+00

- 100% nitrogen, and
- Wet fuel.

Water evaporates until the MCO reaches saturated conditions; i.e., steam partial pressure of 12.349 kPa at 50°C. The validation confirmed that the simulation attained the correct steady-state conditions and calculated the correct evaporation rate at the first time step. The simulation ran for only 100 seconds because conditions became steady after only about 40 seconds. Output at 100 seconds is listed below:

```

Region properties:                                Time=    100.000 seconds
                                                0.028 hours

Timestep =   0.1000      Average =   0.0997

Region # ->          1                      2
Press., Pa          1.135E+05      1.013E+05
Temp., C            4.991E+01      5.000E+01
                  , K            3.231E+02      3.231E+02
Spec. Heat Cv       7.893E+02      7.208E+02
Ratio Cp/Cv         1.392E+00      1.401E+00
k, W/m-C            2.664E-02      2.758E-02
Mole fractions of gas ...
NITROGEN            8.916E-01      7.900E-01
OXYGEN              0.000E+00      2.100E-01
STEAM               1.084E-01      0.000E+00

Gas masses ...
NITROGEN            5.281E-01      8.345E+08
OXYGEN              0.000E+00      2.534E+08
STEAM               4.125E-02      0.000E+00

Relative humidities ...
STEAM               9.953E+01      0.000E+00

Aerosol masses ...

Liquid masses ...

Rates of change of gas and aerosol ...
STEAM              g      2.028E-06      0.000E+00

```

Output shows the correct steady-state response (total pressure and partial pressure of steam), with minor disagreement that can be explained by the non-ideal behavior of water.

The next step was to confirm that at time zero, the evaporation is calculated correctly. This is accomplished using equation (2-18b), which shows the evaporation rate based the

Colburn-Chilton analogy for mass transfer. Values needed to evaluate this equation can be found in the HANSF output and log files. Consider the HANSF output at time zero:

Region properties:

Time= 0.000 seconds
0.000 hours

Timestep = 0.0100 Average = 0.0100

Region # ->	1	2
Press., Pa	1.013E+05	1.013E+05
Temp., C	5.000E+01	5.000E+01
, K	3.231E+02	3.231E+02
Spec. Heat Cv	7.395E+02	7.208E+02
Ratio Cp/Cv	1.403E+00	1.401E+00
k, W/m-C	2.746E-02	2.758E-02

Mole fractions of gas ...		
NITROGEN	1.000E+00	7.900E-01
OXYGEN	0.000E+00	2.100E-01

Gas masses ...		
NITROGEN	5.281E-01	8.345E+08
OXYGEN	0.000E+00	2.534E+08

Relative humidities ...

Aerosol masses ...

Liquid masses ...

Rates of change of gas and aerosol ...		
STEAM g	3.612E-03	0.000E+00

With an MCO volume of 0.5 m³ and 100% nitrogen at 50°C, the following values apply:

k = Thermal conductivity of gas (2.746 x 10⁻³ W/m-C),
 ρ = Gas density (1.0562 kg/m³),
 c_p = Specific heat (1037.5 J/kg-C),
 α = Thermal diffusivity (2.5 x 10⁻⁶ m²/s),
 Y_s = Mass fraction of water at the surface,

$$= \frac{P_{sat} \frac{MW_{H_2O}}{(P - P_{sat}) MW_{N_2} + P_{sat} MW_{H_2O}}}{0.0822},$$

 P_{sat} = Saturation pressure (12.349 kPa),
 P = Total pressure (0.1013 Mpa),
 MW = Molecular wt., and
 Y_∞ = Steam mass fraction in MCO gas (0.0).

The other parameters needed to calculate the evaporation are the heat transfer coefficient (h), the diffusion coefficient (D), and the wetted fuel area. The diffusion coefficient is specified in the HANSF log file:

Compare to diffusion of steam in air at 20C: 0.298E-04 0.600E-04

where 0.2984E-4 m²/s is the value needed, and 0.600E-04 m²/s is the comparison value. Total fuel heat transfer area is about 65 m², but only 10% is wetted, and the wetted area is then 6.5 m². With no temperature gradient, the Nusselt number for heat transfer is not computed based on a Grashof number (which would be zero), but is set to one, signifying pure conduction. That is,

$$h = \frac{k}{\delta} \quad (7-20)$$

where δ is the gap distance. Now the gap distance between inner and outer fuel elements is only 3 mm, while the gap distance between fuel assemblies is a few cm. Therefore, the heat (mass) transfer coefficient is much smaller for the inner surface of the inner fuel element and the outer surface of the outer element. Assuming that half the evaporation area is in the gap between the fuel elements, and half is on the other surfaces, the area-weighted average heat transfer coefficient is,

$$h = k \frac{\frac{1}{\delta_1} + \frac{1}{\delta_2}}{2} \quad (7-21)$$

where δ_1 is the gap between fuel elements (3 mm) and δ_2 is the gap between fuel assemblies (≈ 3 cm). This yields an average heat transfer coefficient of 5.06 W/m²-C.

Evaluating equation (2-18b) gives 3×10^{-3} kg/s, which is in good agreement with the steam rate-of-change at time zero, as shown by the output.

7.9 Hydriding/Dehydriding Validation

To validate the uranium hydride model, run the code with specified MCO conditions and compare hydriding/dehydriding results with hand calculations for the amount of uranium hydride produced/consumed. Input decks used a simplified MCO model that consisted of one fuel assembly, modeled as fourteen heat sinks, and a 1 m³ gas region. Validation required two input decks: one for hydriding, and one for dehydriding.

In the hydriding (formation) validation, initial gas conditions were 200°C and 1 x 10⁵ Pa, with mole fractions of 80% helium and 20% hydrogen. Production and consumption multipliers were set to one, and the total reaction area was 1.21 m². The run lasted 200 seconds.

The hydriding rate law is the Bloch and Mintz correlation described in Section 3.4. With the temperature and partial pressure of hydrogen specified the Bloch and Mintz correlation can be evaluated for the linear velocity of the reaction front. Multiplying the velocity of the reaction front by the reaction area, fuel density, appropriate ratio of molecular weights (241/238), and time gives the uranium hydride production:

$$\Delta M = u \rho_f r A_r \Delta t \quad (7-22)$$

where ΔM = hydride production,

u = Bloch and Mintz velocity (2 microns/min),

ρ_f = fuel density (19,000 kg/m³),

Δt = 200 seconds,

r = 241/238, and

A_r = 1.21 m².

With the specified conditions assumed constant for hand calculation, hydriding produces 0.1631 kg of uranium hydride. This compares to the code calculated value of 0.146 kg. The

minor discrepancy can be explained by the decrease in hydrogen partial pressure that takes place during hydriding and cannot be accounted for in a simple hand calculation.

In the dehydriding (decomposing) validation, initial gas conditions were 200°C and 1×10^5 Pa, with mole fractions of 99% helium and 1% hydrogen. Production and consumption multipliers were set to one, and the total reaction area was 1.21 m². The run lasted 200 seconds. With the specified conditions assumed constant for hand calculation, dehydriding decomposed 0.122 kg of uranium hydride. This compares to the code calculated value of 0.12 kg, which is in excellent agreement.

7.10 Uranium Oxidation Validation

The approach to validating the uranium oxidation model was to run the code with specified MCO gas conditions, and confirm that the uranium oxidation rate matches hand calculations. Four sets of MCO gas conditions were used: (1) 75°C, 1% steam, 20% oxygen, and 79% nitrogen, (2) 300°C, 1% steam, 20% oxygen, and 79% nitrogen, (3) 75°C, 51% oxygen, and 49% nitrogen, and (4) 300°C, 51% steam, and 49% nitrogen. The enclosed MCO consisted of 3 regions with a total volume of 0.56 m³, and 44 heat sinks with a total effective oxidation area of 128 m². No decay heat, evaporation/condensation, or gas heat transfer models were in effect. Cases with 75°C conditions ran for 1000 seconds, and cases with 300°C conditions ran for 1 second.

Validate code results for Case 1 using the Ritchie correlation:

$$m''_{O_2} = 10^{(13.8808 - 5.7696 \times 10^3/T)} \quad (\text{mg/cm}^2\text{-hr}) \quad (7-23)$$

Substituting $T = 348.15$ K into the correlation gives $m''_{O_2} = 5.65 \times 10^{-9}$ kg/m²-sec. With an effective oxidation area of 128 m², the total amount of oxygen consumed during 1000 seconds would be 7.23×10^{-4} kg. This is in excellent agreement with code results that show an

initial oxygen inventory of 0.12138 kg, and an oxygen inventory of 0.12066 kg at 1000 seconds, i.e., oxidation consumed 0.00072 kg of oxygen.

In the same vein, validate the fuel basket temperature rise using a simple energy balance:

$$\Delta T = \frac{m''_{O_2} A Q_r \Delta t}{m_f c} \quad (7-24)$$

where Q_r is the heat of reaction (3.4×10^7 J/kg O_2), A is the oxidation area of one fuel basket (34 m^2), m_f is the fuel mass of one basket (2995.4 kg), c is the fuel specific heat (122.7 J/kg-C), and Δt is the duration of 1000 seconds. Evaluating for ΔT yields 0.018°C , which is consistent with code results that vary between 0.017 and 0.018°C .

These two validation calculations (mass consumption and fuel basket temperature rise) can be repeated for Cases 2, 3, and 4 to obtain the results shown in Table 7-6. The only difference to bear in mind is that the reactions in Cases 3 and 4 consume steam.

Table 7-6: Uranium Oxidation Validation					
Case No.	Correlation (mg/cm ² -hr)	Calculated Mass Consumption (kg)	HANSF Mass Consumption (kg)	Calculated ΔT (°C)	HANSF ΔT (°C)
1	Ritchie $10^{\left(13.8808 - \frac{5.7696 \times 10^3}{T}\right)}$	7.23×10^{-4} (2)	7.2×10^{-4} (2)	0.018	0.017 - 0.018
2	Pearce $10^{\left(6.1931 - \frac{2963}{T} + 0.3 \log\left(\frac{P_H}{1000}\right)\right)}$	0.0143 (4)	0.0144 (4)	0.36	~0.38
3	Pearce $10^{\left(4.33 - \frac{2144}{T} + 0.5 \log\left(\frac{P_H}{1000}\right)\right)}$	0.0423 (2)	0.0403 (2)	0.51	0.47 - 0.50
4	Pearce (Same as in Case 3)	0.0142 (4)	0.0142 (4)	0.17	0.15

- (1) Oxygen in Cases 1 and 2; steam in Cases 3 and 4.
- (2) 1000 seconds duration.
- (3) Each fuel assembly consists of heat sinks with varying fuel temperatures.
- (4) After 1 second.

7.11 Entrainment Validation

An MCO canister initially at 150 psig was allowed to blow down through a 1 inch vent to the environment. The resuspension rate depends on the free stream velocity across the fuel/scrap surface, as shown by

$$\Lambda = 2 \times 10^{-6} U_{\infty}^3 \quad (7-25)$$

where U_{∞} is the free stream velocity and Λ is the resuspension parameter. In the validation, 5.28×10^{-5} kg of sludge particulate were entrained from the initial sludge particle inventory of 142 kg, and 3.5×10^{-5} kg of the resuspended sludge particulate escaped to the environment during the 50 second blow down. Validation by hand calculations follows.

Fuel Basket	Time=0	Time=5	
Mass Flow	0.3048	0.174	kg/s
Area	0.131	0.131	m ²
Density	10.926	6.272	
Velocity (1)			kg/m ³
Sludge Mass	0.213	0.212	m/s
Resuspension Rate	87.6	87.6	kg
Resuspended Mass Rate (2)	1.9E-08	1.90E-08	/s
	1.69E-06	1.66E-06	kg/s

Scrap Basket	Time=0	Time=5	
Mass Flow	0.3048	0.174	kg/s
Radius	0.292	0.292	m
Porosity	0.5	0.5	
Density	10.926	6.272	
Velocity (3)			kg/m ³
Sludge Mass	0.208	0.207	m/s
Resuspension Rate	54.4	54.4	kg
Resuspended Mass Rate (2)	1.81E-08	1.78E-08	/s
	9.83E-07	9.67E-07	kg/s
Total Rate	2.675E-06	2.631E-06	kg/s
(1) Mass Flow / (Area * Density)			
(2) Resuspension * Sludge Mass			
Mass Flow			
(3) $\pi * \text{Porosity} * \text{Radius}^2 * \text{Density}$			

The calculated total resuspension rate of 2.63×10^{-6} kg/s is consistent with the code calculated total aerosol addition rate of 2.634×10^{-6} kg at time = 5 seconds. Since the blow down velocity is essentially constant for the first five seconds, the total accumulated aerosol mass should be $(2.65 \times 10^{-6}) \times (5) \approx 1.33 \times 10^{-5}$ kg which compares well with the code calculated total aerosol mass of 1.316×10^{-5} kg.

7.12 Hydrate Decomposition Validation

To validate the dehydration model, fuel elements were held at about 150°C and the dehydration rates were checked. Dry helium was continuously recirculated through the MCO so that steam partial pressure would not build up in the MCO and limit the dehydration rate. The process was simulated over 100,000 seconds so that the whole sequence encompasses two-step decomposition of uranium hydrate. The first step is decomposition to $\text{UO}_3 \cdot \text{H}_2\text{O}$. The second step is decomposition to $\text{UO}_3 \cdot 0.5\text{H}_2\text{O}$. For this particular validation run, the kinetics

coefficient of the first step (i.e., ADEHY1) is modified to yield ten times the second step decomposition rate. The related section of the input deck is listed below.

```

*
* 10 % weight fraction of sludge being water is equivalent to 90 %
* of sludge being hydrated with 2 moles of
* water per mole of uranium oxide
*
PHYSL 0.9      ! fraction of sludge that is hydrated
XHYSL 2.0      ! stoichiometry number of hydrate: no. of moles of
                ! water per mole of uranium oxide (UO3.H2O)
XHYD2 1.0      ! H2O/U ratio (stoich. number) to switch
                ! from first to second correlation
XHYD3 0.5      ! H2O/U ratio (stoich. number) to switch
                ! from second to third correlation
AHYEQ1 18.012  ! 'A' IN LN P = A + B/T FOR X > XHYD2
BHYEQ1 -6775.E0 ! 'B' IN LN P = A + B/T FOR X > XHYD2
AHYEQ2 19.076  ! 'A' IN LN P = A + B/T FOR X < XHYD2
BHYEQ2 -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD2
AHYEQ3 19.076  ! 'A' IN LN P = A + B/T FOR X < XHYD3
BHYEQ3 -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD3
* ADEHY1 -5.295E0 ! 'A' IN LN K = A + B/T FOR X > XHYD2
ADEHY1 -2.9924E0 ! 'A' IN LN K = A + B/T FOR X > XHYD2
BDEHY1 -2546.E0 ! 'B' IN LN K = A + B/T FOR X > XHYD2
ADEHY2 -5.295E0 ! 'A' IN LN K = A + B/T FOR X < XHYD2
BDEHY2 -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD2
ADEHY3 -5.295E0 ! 'A' IN LN K = A + B/T FOR X < XHYD3
BDEHY3 -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD3
DHHY1 2.86E6    ! Decomposition enthalpy J/kg H2O: 1st step
DHHY2 3.70E6    ! Decomposition enthalpy J/kg H2O: 2nd step
DHHY2 3.70E6    ! Decomposition enthalpy J/kg H2O: 3rd step

```

The code result for the middle fuel basket is summarized below. The fourth column is computed by dividing the third column by the second column.

Time (sec)	Hydrated Sludge Mass (kg)	Water in Sludge (kg)	Fraction of Water in the Sludge
0	40.500	4.528	0.1118
10000	38.979	3.006	0.0771
20000	38.497	2.525	0.0656
30000	38.327	2.355	0.0614
40000	38.267	2.295	0.0600
50000	38.193	2.221	0.0582
60000	39.120	2.148	0.0563
70000	38.033	2.063	0.0542
80000	37.940	1.968	0.0519
90000	37.849	1.877	0.0496
100000	37.768	1.796	0.0476

The target water fraction for the first stage decomposition is $18/(286+18)=0.0592$. Therefore, from the above table, the transition from the first stage to the second stage decomposition occurred between 50,000 and 60,000 sec. The decomposition rate is given by

$$\frac{dM_w}{dt} = -k (M_w - M_t) \quad (7-26)$$

where M_w is the mass of water in the sludge, M_t is the target water mass in the sludge, and k is the kinetics rate multiplier. This can be analytically integrated to

$$M_w = (M_{w0} - M_t) \exp [-k (t - t_0)] + M_t \quad (7-27)$$

where $M_{w0} = M_w(t_0)$.

Target water mass for the first step decomposition is given by

$$(40.500 - 4.528) \frac{18}{286} = 2.264 \text{ kg} \quad (7-28)$$

Target water mass for the second step decomposition is given by

$$(40.500 - 4.528) \frac{9}{286} = 1.132 \text{ kg} \quad (7-29)$$

To validate the first step decomposition, consider $t_0 = 0$ and $t = 10,000$ sec. From above table, $M_{w0} = 4.528$ kg. The average fuel temperature was about 145°C (418 K). Therefore,

$$\begin{aligned} k &= \exp \left(\text{ADEYH1} + \frac{\text{BDEHY1}}{T} \right) \\ &= \exp \left(-2.9924 - \frac{2546}{418} \right) \\ &= 1.14\text{E-}4 \end{aligned} \quad (7-30)$$

Substituting values in equation (7-27) yields,

$$\begin{aligned} M_w &= (4.528 - 2.264) \exp [-1.14\text{E-}4 \times 10,000] + 2.264 \\ &= 2.988 \text{ kg} \end{aligned} \quad (7-31)$$

This agrees with the code calculated amount of water in the sludge at 10,000 sec, 3.006 kg.

To validate the second step decomposition, consider $t_0 = 80,000$ sec and $t = 90,000$ sec. From above table, $M_{w0} = 1.968$ kg. The average fuel temperature was about 145.9°C (419.1 K). Therefore,

$$\begin{aligned} k &= \exp\left(\text{ADEYH2} + \frac{\text{BDEHY2}}{T}\right) \\ &= \exp\left(-5.295 - \frac{2546}{419.1}\right) \\ &= 1.154\text{E-}5 \end{aligned} \quad (7-32)$$

Again, substituting values in equation (7-27) yields,

$$\begin{aligned} M_w &= (1.968 - 1.132) \exp[-1.154\text{E-}5 \times 10,000] + 1.132 \\ &= 1.877 \text{ kg} \end{aligned} \quad (7-33)$$

This agrees with the code calculated amount of water in the sludge at 90,000 sec, 1.877 kg.

7.13 Heat Transfer Validation

Two sets of heat transfer validation cases were considered: 1) fuel to gas heat transfer, and 2) scrap basket heat transfer.

7.13.1 Fuel to Gas Heat Transfer

The model was validated by considering a compartment containing a single fuel basket with 14 heat sinks as MCO fuel. The heat transfer model was tested by specifying a compartment gas temperature, and initializing the heat sinks at a different temperature.

Gas temperature was specified to be 50°C and all the heat sinks, including the MCO wall, were specified to be 500°C . The decay power was set to zero so the only heat transfer

possible is from the heat sinks to the gas. The simulation ran for 500 seconds, but as seen from Figure 7-8, the gas temperature attained steady-state within 15 seconds. For verification, the time constant was calculated. The time constant was calculated as:

$$t = \left(\frac{h A}{\rho V c} \right)^{-1} = \left(\frac{(8) (36.6)}{(0.25) (1) (2963)} \right)^{-1} = 2.53 \text{ seconds} \quad (7-34)$$

where t is the time constant, h is the heat transfer coefficient, A is the heat transfer area, ρ is the gas density, V is the gas volume, and c is the heat capacity of the gas. The value for heat transfer coefficient, h , is an estimate based on natural convection and radiation to the gas; other values are inputs to the case. The calculated time constant is consistent with the rate of gas temperature increase as shown in Figure 7-8.

7.13.2 Scrap Basket Heat Transfer

Validate the scrap basket heat transfer model by comparing the code-calculated peak temperature with the analytically calculated peak temperature. The run used for this comparison assumes: (1) the scrap is initially at 50°C, (2) the fin is maintained at 50°C, (3) heat transfer to the gas, oxidation, evaporation, and dehydration models are neglected. The MCO model consisted of 3 regions and 44 heat sinks; 1 scrap basket tier and 4 fuel basket tiers were modeled as 2 fuel baskets. A single scrap basket was described by a 30 degree sector: the radius of the basket is 0.286 m, the coarse region starts from 0.09652 m, the fine region is subdivided into interior and exterior regions, with exterior region starting at 0.06081 m. Volumetric heat generation was 2131 W/m³. Porosity was 0.45 in the fines, and 0.60 in the coarse scrap.

The peak temperatures in the interior fine region and in the exterior coarse regions are compared with analytical solution. The peak temperature in the coarse region occurs in the inner surface of the exterior region and is given by:

$$T_{\max, \text{ext}} - 50.052^\circ\text{C} = Q \frac{R^2}{4k} \left[1 - \left(\frac{a}{R} \right)^2 + 2 \left(\frac{a}{R} \right)^2 \ln \frac{a}{R} \right] \quad (7-35)$$

Figure 7-8: Gas Temperature for Heat Transfer Validation.

where Q is the bulk volumetric heat generation rate, R is the radius of the basket, k is the effective thermal conductivity, and ' a ' is the radial distance of the inner surface of the exterior region. Therefore,

$$\begin{aligned}
 T_{\max, \text{ext}} - 50.052^{\circ}\text{C} &= 2131 (1 - 0.6) \frac{0.286^2}{4 \cdot 1.41} \\
 &\quad \cdot \left[1 - \left(\frac{0.19126}{0.286} \right)^2 + 2 \left(\frac{0.19126}{0.286} \right)^2 \ln \frac{0.19126}{0.286} \right] \quad (7-36) \\
 &= 2.38^{\circ}\text{C}
 \end{aligned}$$

This agrees with the code calculated maximum temperature rise in the exterior coarse region of 2.40°C .

The peak temperature in the fine interior region occurs in the inner-most surface node of the second ring. The analytical solution is given by:

$$T_{\max, \text{int}} - 50.052^{\circ}\text{C} = Q r^2 \frac{\theta^2}{2k} \quad (7-37)$$

where ' r ' is the radial distance of the mid-point of the third ring and θ is the angular distance of the inner-most node from the fin. Therefore,

$$\begin{aligned}
 T_{\max, \text{int}} - 50.052^{\circ}\text{C} &= 2131 (1 - 0.45) 0.046^2 \frac{\left(\frac{\pi}{6} \right)^2}{2 \cdot 1.15} \quad (7-38) \\
 &= 0.30^{\circ}\text{C}
 \end{aligned}$$

This is somewhat lower than the code calculated maximum temperature rise of 0.41°C . The discrepancy is expected because the planar heat sink assumption breaks down when the annulus is close to the center.

In order to check that the code changes related to sub-dividing the scrap basket heat sinks into interior and exterior regions do not affect other calculations (other than heat transfer, such as corrosion, evaporation, etc.), the previous case was run with the corrosion model turned on. A maximum temperature rises of 4.823°C in the coarse region was obtained. Without the

corrosion model turned on, the resulting peak temperature rises was 3.390°C. Hence, the temperature rise increased by about 42% when the corrosion model was turned on.

Using a debugger, the corrosion heat in the Heat Sink-37 was examined to be

$$QCORRD(37,2) = 12.78 \text{ W} \quad (7-39)$$

On the other hand, the decay heat in the Heat Sink-37 is given by,

$$2131 (1 - 0.6) 0.03446 \text{ m}^3 = 29.33 \text{ W} \quad (7-40)$$

Therefore, we expect increase in the peak temperature by $12.75 / 29.33 = 43\%$, which is consistent with 42% predicted by the code.

7.14 Nitriding Validation

The approach to nitriding model validation was to run the code with specified MCO gas conditions and confirm that the nitriding rate matches hand calculations. The enclosed MCO consisted of 3 regions with a total volume of 0.56 m³, and 44 heat sinks with a total effective reaction area of 11.4 m². To encompass the different nitriding rate law regimes, three temperatures were employed: (1) 700°C, (2) 760°C, and (3) 800°C. Initial gas and heat sink temperatures were set equal to the temperature for the particular case. The MCO atmosphere was initially 90% nitrogen and 10% helium. Case 1 ran for 1000 seconds, while Cases 2 and 3 ran for 100 seconds.

Integrating the parabolic rate law gives:

$$W_{N_2}^2 = k(T) t \quad (7-41)$$

where W_{N_2} is the weight gain of nitrogen per unit area, $k(T)$ is the rate constant $((\text{ml}/\text{cm}^2)^2/\text{s})$, measured at STP), and t is time in seconds. Total nitrogen consumption is then:

$$\Delta M_{N_2} = A \sqrt{c k(T) t} \quad (7-42)$$

where A is the effective reaction area, and c is a conversion factor $(1.3 \times 10^{-4} \text{ kg}/\text{m}^2\text{-s})$. Rate laws are listed in Section 3.13.

Table 7-7 shows a comparison of hand calculations with HANSF results, and demonstrates proper code functioning.

Table 7-7: Nitriding Validation					
Case #	T (°C)	t (seconds)	k (T)	N ₂ Consumption	
				Code	Hand Calculation
1	700	1000	3.79×10^{-4}	0.084	0.083
2	760	100	1.55×10^{-3}	0.077	0.077
3	800	100	3.32×10^{-3}	0.054	0.053

7.15 Pump Model

Pump model validation uses a sequence that simulates the helium gas recirculation cycle following the vacuum cycle. In this sequence, the pump model is activated to simulate the recirculation pump, condenser, and the feed. Then, a junction is connected between the MCO and the environment to simulate the bleed. Input parameters related to the pump model are as follows:

-
- * PUMP, FEED, AND CONDENSER MODELS
- * Syntax:
- * PUMP IRIPIUM IROPUM ICONPM ITFEED WVPUMP WVFEED TGFEED TCONPM
- *

* Definitions:

* IRIPUM - Pump inlet region
 * IROPUM - Pump outlet region
 * ICONPM - Node to which the condensed steam is dumped for book-keeping
 * ITFEED - If non-zero, overrides TGFEED with the designated region
 • temperature. Used to specified time-varying feed temperature
 * WVPUMP - Pump volumetric flowrate (m³/s)
 * WVFEED - Feed volumetric flowrate (m³/s)
 * TGFEED - Feed temperature (K)
 * TCONPM - Condenser cooling coil temperature (K)
 *
 • 10 FT³/MIN * 1 MIN/60 SEC * 0.02832 M³/1 FT³ = 0.00472 M³/SEC
 * PUMP IRIPUM IROPUM ICONPM ITFEED WVPUMP WVFEED TGFEED TCONPM
 PUMP 1 3 5 0 0.00472 0.000944 50.0 1.5

Using the debugger, the pump model was checked to verify that at 5000 seconds: (1) the gas was removed at the user-specified volumetric flowrate, (2) the steam mole fraction of the returning gas was reduced to the saturation value at the user-specified condenser temperature, (3) the makeup helium flow was correctly added to the recirculating gas flow, and (4) the makeup helium flow was correctly added to the recirculating gas flow.

The expected mass flow rate leaving the MCO top volume is a product of volumetric flow rate and density in Volume 1:

$$0.00472 \text{ m}^3/\text{sec} \cdot 0.2177 \text{ kg/m}^3 = 0.00103 \text{ kg/sec.} \quad (7-43)$$

The debugger reported the following rates-of-change in gas mass (RMG):

RMG(1,1) = - 0.13717E-6, nitrogen
 RMG(2,1) = 0.00000E+0, oxygen
 RMG(3,1) = - 0.412481E-3, steam
 RMG(4,1) = - 0.328375E-5, hydrogen
 RMG(5,1) = - 0.611981E-3, helium

The sum of these three rates gives 0.001028 kg, consistent with the expected mass flow rate leaving the node-1.

Consider the condensation rate next. According to equation (5-13), the fraction of steam flow condensed, f , is

$$f = 1.0 - \text{Min} \left\{ 1.0, \frac{P_c}{P_{st}} \right\} \quad (7-44)$$

where P_c is the saturation pressure at TCONPM and P_{st} is the steam flow partial pressure. For the user-specified condenser cooling coil temperature (1.5°C), P_c is 685 Pa. Steam flow partial pressure is the steam mole fraction multiplied by the total pressure. From the debugger,

$$P_{st} = (0.129) (101,200) \text{ Pa} = 13,055 \text{ Pa} \quad (7-45)$$

Condensation rate should be,

$$\begin{aligned} W_c &= \text{WVPUMP} \cdot \left(1 - \frac{685}{13,055} \right) x_{st} \rho_{\text{donor}} \\ &= \text{WVPUMP} \cdot 0.9476 x_{st} \rho_{\text{donor}} \end{aligned} \quad (7-46)$$

where ρ_{donor} is gas density in the donor volume and x_{st} is the steam mass fraction. Then,

$$\begin{aligned} W_c &= \left(0.00103 \frac{\text{kg}}{\text{s}} \right) (0.401) (0.9476) \\ &= 3.913 \cdot 10^{-4} \frac{\text{kg}}{\text{s}} \end{aligned} \quad (7-47)$$

The steam flow rate to the MCO bottom should then be,

$$\begin{aligned} W_{st} &= \left(0.00103 \frac{\text{kg}}{\text{s}} \right) (0.401) (1 - 0.9476) \\ &= 2.16 \cdot 10^{-5} \frac{\text{kg}}{\text{s}} \end{aligned} \quad (7-48)$$

which is agreement with the debugger volume of $1.90 \times 10^{-5} \text{ kg/s}$.

The user-specified helium feed rate was $0.000944 \text{ m}^3/\text{sec} \times 0.15 \text{ kg/m}^3 = 1.419\text{E-}4 \text{ kg/sec}$. This is consistent with the observed rate-of-change in helium gas mass in the environment node, $\text{RMG}(5,5) = 1.421\text{E-}4$.

MCO pressure was maintained constant at 101,200 Pa and the gas temperature remained at 323 K, while the pump was running.

7.16 Radiation Network Validation

The radiation network facility was validated by comparison with a problem amenable to hand calculation [Incropera and DeWitt, 1981]. Consider a radiation network made up of three surfaces that form an enclosure. Each surface as a unique area, emissivity, and temperature, as follows:

$$\begin{array}{lll} T_1 = 1000 \text{ K}, & T_2 = 600 \text{ K}, & T_3 = 300 \text{ K}, \\ \epsilon_1 = 0.9, & \epsilon_2 = 0.5, & \epsilon_3 = 1.0, \\ A_1 = 10.0 \text{ m}^2, & A_2 = 15.0 \text{ m}^2, & A_3 = 22.0 \text{ m}^2. \end{array}$$

and a view factor matrix is,

$$\begin{array}{lll} F_{11} = 0.0 & F_{12} = 0.39 & F_{13} = 0.61 \\ F_{21} = 0.26 & F_{22} = 0.33 & F_{23} = 0.41 \\ F_{31} = 0.28 & F_{32} = 0.28 & F_{33} = 0.44 \end{array}$$

Hand calculation shows that the heat transfer rate to the second heat sink is -77.7 kW [Incropera and DeWitt, 1981].

The parameters shown above were used for a HANSF input file. At the first time step, the heat transfer rate to the second heat sink was found from a debugger session record:

```
QVIEWNW=
-463954.
77505.8 ←
386447.
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
```

Variable QVIEWNW is the net radiation heat transfer from each heat sink, in W. Ten heat sinks are allowed in a radiation network, at most, which explains why the last seven QVIEWNW values are zero. Note that the hand calculation uses a reverse sign notation relative to the code, but the magnitudes are very close. Also, the sum of the heat transfer rates shown in the debugger session is only 1.2 W. Net heat transfer should be zero for an enclosure, but the value of 1.2 W is very small relative to the magnitudes of the individual heat transfer rates and shows that the code is essentially conserving energy.

These initial conditions cannot persist without heat sources or prescribed boundary conditions. In the HANSF input file, no heat sources nor prescribed boundary conditions were included, which allowed the heat sinks to equilibrate. Convection was negated and the heat sinks exchanged energy only via the radiation network. Each heat sink had the same set of thermophysical properties and thickness. Therefore, the final temperature, T_f , must be an average based on the heat sink areas:

$$T_f = \frac{\sum_{i=1}^3 T_i A_i}{\sum_{i=1}^3 A_i} \quad (7-49)$$

where A_i is the area of heat sink i and T_i is the initial temperature of heat sink i . This equals 271.5°C. After 50,000 seconds, the output file shows good agreement with the expected result:

Heat sink temperatures:				Time= 50000.000 seconds 13.889 hours				
HS # 1	(	insulated	)	271.504	271.504	271.504	271.504	271.504
		271.504	271.504	271.504	271.504	271.504	271.504	271.504
		271.504	271.504	271.504	271.504	271.504	271.504	271.504
		271.504	(	insulated	)			
HS # 2	(	insulated	)	271.504	271.504	271.504	271.504	271.504
		271.504	271.504	271.504	271.504	271.504	271.504	271.504
		271.504	271.504	271.504	271.504	271.504	271.504	271.504
		271.504	(	insulated	)			
HS # 3	(	insulated	)	271.503	271.503	271.503	271.503	271.503
		271.503	271.503	271.503	271.503	271.503	271.503	271.503
		271.502	271.502	271.503	271.503	271.503	271.503	271.503
		271.502	(	insulated	)			

7.17 Energy Balance Validation

A simple MCO transient heat-up was run to validate HANSF ability to conserve energy. The idea was to make a run with decay heat as the only source and verify that at steady-state, decay heat equals losses to the MCO wall. This run incorporated the following features:

- Seven regions: Region 1 was the scrap basket, Regions 2 – 5 were the four fuel baskets, Region 6 was the gap between MCO and cask, and Region 7 was the environment.
- Seventy-four heat sinks represented the scrap and fuel baskets,
- No junction nor counter-current flows; no helium purge nor vacuum pumping,
- No water nor hydride,
- No oxidation, evaporation, nor condensation,
- No diversion of heat to MCO gas,
- Volumetric heat generation at 1957.0 W/m^3 , for a total decay power of 733 W,
- All initial temperatures at 50°C ,
- MCO wall temperature fixed at 50°C , and
- Five million seconds as an arbitrary, very long time.

In the process of validating the energy balance, it was useful to check the print out of mass and heat capacity inventories. Heat capacities were validated by hand calculation, per the following equation:

$$MC = \rho_{HS} V_{HS} c_{HS} \quad (7-50)$$

Inputs for ρ_{HS} , V_{HS} , and c_{HS} are as follows:

- Cask wall: $\rho_{HS} = 7753 \text{ kg/m}^3$, $V_{HS} = 1.902 \text{ m}^3$, and $c_{HS} = 486.0 \text{ J/kg-C}$,
- Lid/floor: $\rho_{HS} = 8000 \text{ kg/m}^3$, $V_{HS} = 0.097 \text{ m}^3$, and $c_{HS} = 500.0 \text{ J/kg-C}$,
- MCO wall: $\rho_{HS} = 8000 \text{ kg/m}^3$, $V_{HS} = 0.07 \text{ m}^3$, and $c_{HS} = 500.0 \text{ J/kg-C}$, and
- Scrap basket fin: $\rho_{HS} = 8954 \text{ kg/m}^3$, $V_{HS} = 0.0084 \text{ m}^3$, and $c_{HS} = 384.0 \text{ J/kg-C}$.

For each heat sink, volume is computed by the product of thickness ($XRO - XRI$) and area (AHS). MCO wall and lid/floor are made up of more than one heat sink. These inputs result in heat capacities as follows:

- Cask wall: $7.166 \times 10^6 \text{ J/C}$,
- Lid/floor: $3.880 \times 10^5 \text{ J/C}$,
- MCO wall: $2.80 \times 10^5 \text{ J/C}$, and
- Scrap basket fin: $2.888 \times 10^4 \text{ J/C}$.

The above calculations can be compared to HANSF output at time zero:

MCO/Cask structure heat capacities (J/C):

cask wall	7.165E+06
lid/floor	3.886E+05
MCO wall	2.794E+05
insert	0.000E+00
scrap bskt fin	2.883E+04

The MCO print out lists various masses, areas, and all the elements of the fuel energy balance, including decay heat. To verify that the decay heat is correct, first compute the mass of fuel in one fuel basket. Consider heat sinks 16 through 29, which together constitute one fuel basket. The following Table 7-8 computes the mass of fuel in one fuel basket. Note that XRO, XRI, and AHS are inputs, and VOLHS and MASS-HS are calculated according to the following:

$$VOLHS = (XRO - XRI) AHS, \quad (7-51a)$$

and

$$MASS-HS = VOLHS * RHO \quad (7-51b)$$

where RHO is the fuel density of 17210 kg/m^3 . This calculation approximates heat sinks as slabs.

Table 7-8: Mass of Fuel in One Fuel Basket

# →	16	17	18	19	20	21	22
XRO	0.01625	0.03075	0.01625	0.03075	0.01625	0.03075	0.01625
XRI	0.0061	0.0216	0.0061	0.0216	0.0061	0.0216	0.0061
AHS	0.278	0.655	0.278	0.655	0.278	0.655	0.577
VOLHS	0.00282	0.00599	0.00282	0.00599	0.00282	0.00599	0.00585
MASS-HS kg	48.5614	103.143	48.5614	103.143	48.5614	103.143	100.791
# →	23	24	25	26	27	28	29
XRO	0.03075	0.01625	0.03075	0.03075	0.03075	0.03075	0.03075
XRI	0.0216	0.0061	0.0216	0.0216	0.0216	0.0216	0.0216
AHS	1.31	0.278	0.655	0.278	0.655	0.557	1.31
VOLHS	0.01198	0.00282	0.00599	0.00254	0.00599	0.00509	0.01198
MASS-HS kg	206.287	48.5614	103.143	43.7770	103.143	87.7116	206.287
TOTAL kg	1354.82						

Decay heat is then $(1354.82 / 17210) * 1957 \text{ W} = 154.1 \text{ W}$, where 1957 is the volumetric heat generation in W/m^3 .

This calculation can be compared to the MCO printout at time zero:

mass inventories:	Time=	0.000 seconds	0.000 hours	MCO
	fuel basket 1	fuel basket 2	fuel basket 3	
uranium mass (kg)	1357.127	1357.127	1357.127	
oxide mass (kg)	0.000	0.000	0.000	
hydride mass (kg)	0.142	0.142	0.142	
dehydrided hydride mass (kg)	0.000	0.000	0.000	
nitride mass (kg)	0.000	0.000	0.000	
water on fuel (kg)	0.101	5.999	0.000	
sludge mass (kg)	5.200	5.200	5.200	
hydrated sludge mass (kg)	0.901	0.901	0.901	
water in sludge (kg)	0.101	0.101	0.101	
heat capacity of fuel (J/C)	176848.	201500.	176426.	
water on insert (kg)	0.000	0.000	0.000	
water on MCO (kg)	0.000	0.000	0.000	
fuel exposed area (m^2)	0.875	0.875	0.875	
fuel oxidation area (m^2)	8.752	8.752	8.752	
hydride oxidation area (m^2)	10.502	10.502	10.502	
MCO wall area (m^2)	1.100	1.100	1.100	
decay power (W)	155.297	155.297	155.297	

Comparison of hand calculations and the code output shows that fuel mass and decay heat are in good agreement, with a slight error in the hand calculation that can be attributed to approximating the cylindrical heat sinks as planar slabs; the code calculates the volume of the cylindrical slab explicitly.

At five million seconds, a printout of the energy balance is:

	fuel basket 1	fuel basket 2	fuel basket 3
uranium mass (kg)	1357.127	1357.127	1357.127
oxide mass (kg)	0.000	0.000	0.000
hydride mass (kg)	0.142	0.142	0.142
dehydrided hydride mass (kg)	0.000	0.000	0.000
nitride mass (kg)	0.000	0.000	0.000
water on fuel (kg)	0.101	5.999	0.000
sludge mass (kg)	5.200	5.200	5.200
hydrated sludge mass (kg)	0.901	0.901	0.901
water in sludge (kg)	0.101	0.101	0.101
heat capacity of fuel (J/C)	176848.	201500.	176426.
water on insert (kg)	0.000	0.000	0.000
water on MCO (kg)	0.000	0.000	0.000
fuel exposed area (m ²)	0.875	0.875	0.875
fuel oxidation area (m ²)	8.752	8.752	8.752
hydride oxidation area (m ²)	4.201	4.201	4.201
MCO wall area (m ²)	1.100	1.100	1.100
decay power (W)	155.297	155.297	155.297
oxidation power (W)	0.000	0.000	0.000
nitriding power (W)	0.000	0.000	0.000
hydriding power (W)	0.000	0.000	0.000
rad/conv loss to MCO wall(W)	155.297	155.298	155.298
rad loss to lid/floor (W)	0.000	0.000	0.000
conv loss to gas (W)	0.000	0.000	0.000
evap/dehyd/radioly loss (W)	0.000	0.000	0.000
cond loss to other hs (W)	0.000	0.000	0.000
	fuel basket 4	scrap basket 1	MCO total
uranium mass (kg)	1357.127	980.742	6409.249
oxide mass (kg)	0.000	0.000	0.000
hydride mass (kg)	0.142	0.730	1.297
dehydrided hydride mass (kg)	0.000	0.000	0.000
nitride mass (kg)	0.000	0.000	0.000
water on fuel (kg)	0.000	0.000	6.099
sludge mass (kg)	0.000	0.000	15.600
hydrated sludge mass (kg)	0.000	0.000	2.702
water in sludge (kg)	0.000	0.000	0.302
heat capacity of fuel (J/C)	176426.	127496.	858698.
water on insert (kg)	0.000	0.000	0.000
water on MCO (kg)	0.000	0.000	0.000
fuel exposed area (m ²)	0.875	4.503	8.004
fuel oxidation area (m ²)	8.752	45.032	80.039

hydride oxidation area (m ²)	4.201	21.616	38.419
MCO wall area (m ²)	1.100	1.100	5.500
decay power (W)	155.297	112.227	733.417
oxidation power (W)	0.000	0.000	0.000
nitriding power (W)	0.000	0.000	0.000
hydriding power (W)	0.000	0.000	0.000
rad/conv loss to MCO wall(W)	155.297	112.790	733.980
rad loss to lid/floor (W)	0.000	-0.154	-0.154
conv loss to gas (W)	0.000	0.000	0.000
evap/dehyd/radioly loss (W)	0.000	0.000	0.000
cond loss to other hs (W)	0.000	0.000	0.000

In regard to the energy balance at five million seconds:

- Energy balances for the individual tiers are in excellent agreement; agreement is virtually perfect for the fuel baskets.
- Overall, the MCO fuel energy balance is good: decay power is equal to 733.417 W and losses are equal to 733.826 W, which is an error of only 0.06%.
- This energy balance not only confirms the printout facility, but also validates HANSF models for heat transfer in the fuel assembly array and scrap basket, heat transfer from the scrap to the fin, and heat transfer from the scrap baskets and fuel assemblies to the MCO walls and lid/floor.

8.0 INTEGRAL TESTING

Four integral tests illustrate use of the code for typical MCO transients and demonstrate reasonable performance consistent with expectation: (1) nominal simulation of the cold vacuum drying (CVD) process, (2) shipping simulation, (3) interim storage, and (4) cold vacuum drying with axial variation in fuel damage. Input decks for these cases are in Appendix B and results are plotted in Appendix C.

In the first three integral tests, the MCO configuration has a single scrap basket loaded into the top tier. The basket has copper fins, as described in Section 3 and illustrated in Figure 3-5. The MCO is nodalized with three control volumes, where the top node contains the scrap tier and the other nodes each contain two lumped fuel baskets. In the fourth integral test, the MCO is nodalized with five control volumes as in Figure 3-6, where the top node contains the scrap tier and each of the other nodes contains a fuel basket tier. Also, the fuel baskets are partitioned into seven segments, with damage limited to the fuel element top segment.

8.1 Cold Vacuum Drying

The first integral test is the normal operation of vacuum pump drying. Two regions are used for the MCO exterior, one for the gap between the MCO and the cask, and another for the environment. Key features are:

1. A vacuum pump draws gas at 35 scfm from a just-drained MCO, and there is a helium addition of 2.5 scfm.
2. Bounding power and oxidation reaction values are used, as listed in Table 8-1.
3. Hydrogen reactions with fuel (gettering) are neglected. This maximizes the hydrogen yield from steam-uranium reactions.
4. All fuel and structure temperatures are initially 50°C.

**Table 8-1:
Simulation Input Values for Integral Test Case 1.**

Decay Power	770 W/MCO (bounding)
Scrap Mass	980 kg
Fuel Mass (per basket)	1498 kg
Scrap Reaction Area	6 m ² (bounding)
Fuel Reaction Area (all)	7 m ² (bounding)
Reaction Rate Law	Literature x 10 (bounding)
Hydride Rate Contribution	Literature x 12 (bounding)
Scrap Water Inventory (CVD)	1.5 kg
Fuel Water Inventory (CVD)	24 kg
Scrap Hydrate Water	0.41 kg (bounding)
Fuel Hydrate Water	0.40 kg (bounding)
MCO Free Volume	0.5 m ³
Fuel Emissivity	0.7
MCO Emissivity	0.25
Pump Flow Rate (CVD)	35 cfm
Helium Injection (CVD)	2.5 cfm

5. The water-filled annulus is represented by a "gas" that has water thermal properties.
6. The cask and MCO external wall temperatures are fixed using the imposed heat sink temperature capability.
7. The case is purposely run for 2 days (172,800 seconds) to allow observation of system behavior, even though process times and operator interventions would limit the duration of real sequences.
8. No axial variations in fuel or scrap baskets.

Other details are included in Table 8-1, which shows basic input values for this integral test run.

Results (see Appendix C) demonstrate that during vacuum pumping with a limited source of water, fuel temperatures remained low and fuel oxidation and hydrogen generation are limited. This is of particular interest because the low thermal conductivity of steam raises the question of whether or not heat can be effectively rejected by the scrap basket. In this case, free water was evaporated at about 14 hours (50,000 seconds), and over the whole transient about 28 kg of water and 0.07 kg of hydrogen were removed. Early in the process, temperatures throughout the MCO decline due to evaporative cooling. Fuel temperatures exhibit a pattern of cooling followed by reheat as a dryout front moves inward from the MCO wall. Long-term steady-state temperatures are attained after about one day in the scrap basket because of the low heat transfer resistance compared to the fuel baskets.

8.2 Shipping Calculation

The second integral calculation is a million-second (11.5 days) shipping calculation. The motivation for such a run is to establish an MCO shipping interval that maintains pressure and temperature within stable and acceptable conditions. The same nodalization is used as with the vacuum drying case. Key differences from vacuum drying are:

1. The MCO is sealed.

2. Helium is the fill-gas between the MCO and the cask.
3. The water inventory reflects loss of free water and partial decomposition of hydrates at CVD.
4. Solar radiation strikes the cask wall and lid.
5. The environment has a diurnal temperature variation for the "hottest Hanford Site day".
6. Shipping begins at noon.

Appendix C shows MCO pressure during the shipping interval. Because the maximum permissible MCO pressure is 1 MPa (150 psig), the figure shows that a safe shipping interval is at least 11.5 days.

Input is set so that the first decomposition step is $1.2\text{H}_2\text{O}\cdot\text{UO}_3 \rightarrow 0.8\text{H}_2\text{O}\cdot\text{UO}_3$, which means that the hydrate would lose 0.05 ($0.144 \text{ kg} \times 0.4 / 1.2$) kg of water during the first step. Output shows at 200,000 seconds, the first decomposition step is complete and the second ($0.8\text{H}_2\text{O}\cdot\text{UO}_3 \rightarrow 0.5\text{H}_2\text{O}\cdot\text{UO}_3$) is about to begin. Hydrate decomposition is much slower during the second step, however, because of constants in the decomposition rate constant. Decomposition rate is:

$$\frac{dM_w}{dt} = -K(T) (M_w - M_w^*) \quad (8-1)$$

where M_w is the mass of hydrate water, $K(T)$ is the temperature-dependent rate constant, and M_w^* is the target mass of hydrate water. The rate constant can be expressed as

$$K(T) = \exp \left(A + \frac{B}{T} \right) \quad (8-2)$$

where $K(T)$ is in inverse seconds, and the decomposition time constant is:

$$\tau = \frac{0.693}{K(T)} \quad (8-3)$$

Assume the fuel/scrap basket temperature is 350 K. With A and B equal to 2.793 and -5111.0, respectively, for the first step and 6.348 and -7241.0, respectively, for the second step. τ equals roughly 93,000 seconds for the first step and over a million seconds for the second step. We would expect the first decomposition step to go to completion, but not the second.

The important point here is that limitations on hydrate decomposition prevent thermal excursions in the MCO. Code results show that temperatures in the MCO reach a steady maximum of about 120°C, with small oscillations attributed to the diurnal cycle.

8.3 Interim Storage

Interim storage at a high temperature location in the CSB vault was simulated for an MCO with the bounding decay power (770 W), nominal water inventory (0.144 kg uranium oxide hydrate), and nominal reactive surface area (see Table 8-1). A CSB vault temperature of 62°C is the given boundary condition, and using vault parameters from the CSB thermal analysis [Flour Daniel, 1996], a vault tube temperature of 92°C and MCO wall temperature of 108°C are derived for the bounding case. The CSB-vault tube gap is 0.6" of air.

Steady-state temperatures are achieved in about 2.5 days, and nearly all the uranium oxide hydrate that can decompose at CSB temperatures is in fact decomposed. From the model employed, 25% of the hydrate water should remain because it requires higher temperatures for decomposition, leading to a mass fraction of about 3% still available for radiolysis. Decomposition goes about to this point for the hottest portion of the fuel in the bounding case, and not quite to this point for the coolest portion, the scrap. About 3.2% water remains in the fuel and about 4.2% in the scrap, with decomposition still slowly progressing.

An MCO pressure of 1.84 atm is attained. The actual pressure of an MCO over a longer time interval depends upon the relative rates of radiolysis of the remaining uranium oxide hydrate and any cladding surface film, such as $Al(OH)_3$ if present, versus the rate of gettering of oxygen and hydrogen. Fuel temperatures are between 122°C and 139°C after 5 days.

8.4 Cold Vacuum Drying With Axial Variation in Fuel Damage

This run is similar to the cold vacuum drying run described in Section 8.1. Key features 1 - 6 from Section 8.1 are still used, but simulation values are as shown in Table 8-2. The intent was to determine if an uneven distribution of free water and reactive area leads to a thermal excursion. Other notable differences are:

- The MCO is nodalized with five control volumes, where the top node contains the scrap basket and each of the other nodes contains a fuel basket. Also, the fuel baskets are partitioned into seven segments, with damage limited to the fuel element top segment. The scrap basket is partitioned into four segments, with most of the water in the bottom 2" of the scrap basket.
- The insert has been included as part of the radiation and gap conduction networks.
- Fuel baskets have been partitioned axially according to the following proportions: 5.21% (top), 4.25%, 6.48%, 9.95%, 15.2%, 23.4%, and 35.51% (bottom). Partitioning is finer near the damaged end to capture expected axial temperature gradients. All reactive area, hydride, and free water content are limited to the top segment. Sludge is evenly distributed axially. The top fuel basket has only 0.1 kg of free water, while the other three have 6 kg each.
- The scrap basket has been partitioned axially according to the following proportions: 30.83%, 30.83%, 30.83%, and 7.51% (bottom). Porosity, reactive area, and scrap size are axially uniform. Free water is distributed with 1 kg on the bottom node, and 0.167 on each of the top three nodes.

Results (see Appendix C) show that temperatures remain low and that oxidation and hydrogen generation are limited, and that axial variations in reactive area and free water do not necessarily lead to thermal excursions. For brevity, results are presented for one tier from the scrap and one tier from each of the four fuel baskets. For the three lower fuel baskets water was evaporated over about 14 hours, as in the first integral test case; the three lower fuel baskets each contained 6 kg of water. In the top fuel basket, which contained only 0.1 kg, dried out after only an hour or so. Fuel temperatures show a pattern of cooling as the evaporation occurs and reheating following the dryout. As a result, the top fuel basket exhibited the highest fuel temperatures after one day. Fuel elements near the insert reached about 79°C.

Table 8-2:
Simulation Input Values for Integral Test Case 4.

Decay Power	770 W/MCO (bounding)
Scrap Mass	980 kg
Fuel Mass (per basket)	1357 kg
Scrap Reaction Area	4.5 m ² (bounding)
Fuel Reaction Area (all)	3.5 m ² (bounding)
Reaction Rate Law	Literature x 10 (bounding)
Hydride Rate Contribution	Literature x 12 (bounding)
Scrap Water Inventory (CVD)	1.5 kg
Fuel Water Inventory (CVD)	19.5 kg
Scrap Hydrate Water	0.41 kg (bounding)
Fuel Hydrate Water	0.40 kg (bounding)
MCO Free Volume	0.5 m ³
Fuel Emissivity	0.7
MCO Emissivity	0.25
Pump Flow Rate (CVD)	35 cfm
Helium Injection (CVD)	1.6 cfm

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APPENDIX A
INPUT DECKS FOR SEPARATE EFFECTS

A.1 Region Thermodynamics Validation Test

A.1 Region Thermodynamics Validation Test

C ENTER: TIME, TEMP, FLOWRATES, POWER
C SYNTAX EXAMPLE:
REGION 1 GASES 1
STEAM
0.0 26.85 0.0 85.74E3
10.0 26.85 0.0 85.74E3
10.02 26.85 0.0 0.0
20.02 26.85 0.0 0.0
END REGION
REGION 2 GASES 1
STEAM
0.0 26.85 0.0 185.79E3
10.0 26.85 0.0 185.79E3
10.02 26.85 0.0 0.0
20.02 26.85 0.0 0.0
END REGION
REGION 3 GASES 1
STEAM
0.0 26.85 0.0 530.6E3
10.0 26.85 0.0 530.6E3
10.02 26.85 0.0 0.0
20.02 26.85 0.0 0.0
END REGION
END SOURCE
END CONTROL ! End of CONTROL keyword group

VOLUMES 3 ! total number of control volumes
VOLUME m⁻³, SED_AREA m⁻², ELEVATION m, TEMP GAS C, PRESSURE Pa
REGIONS 1 2 3
VOLUME 1.000 1.000 1.000
SED_AREA 0.000 0.000 0.000
ELEVATION 0.000 0.000 0.000
TEMP GAS 144.85 144.85 144.85
PRESSURE 4.600E5 4.600E5 4.600E5
END REGIONS ! REGIONS is a comment

TITLE ! Keyword; next line is title, title can be any length
Constitutive Relation Validation Test
END TITLE ! Anything after END is a comment
TIMING ! Keyword
TSTART 0. ! RESTART FILE IS READ FROM HANSFERRER
TLAST 10.1 ! END TIME (Seconds)
DTMIN 0.0 0.05 ! MIN TIMESTEP (Seconds)
DTMAX 0.0 0.05 ! MAX TIMESTEP (Seconds)
DTPRN 0.0 2.0 ! PRINT INTERVAL (Seconds)
PLTMN 0.0 10.1 ! MIN PLOT INTERVAL WITHOUT PLOT (Seconds)
PLTMX 0.0 10.1 ! MAX INTERVAL WITHOUT PLOT (Seconds)
DTRST 0.0 10.1 ! RESTART INTERVAL (Seconds)
FTPC 0.005 ! FRACTIONAL CHANGE IN T AND P
FAECH 0.005 ! FRACTIONAL CHANGE IN AEROSOL MASS
FPFLCH 0.03 ! FRACTIONAL CHANGE FOR PLOTTING
END TIMING ! TIMING is a comment.
ACTIVE MODELS ! Keyword; MODELS is a comment; 1 = on, 0 = off
IUNC 0 ! Junction flow model
ICELW 0 ! Counter-current flow model
IRHSK 0 ! Heat sinks
ICNDS 0 ! Condensation
IALED 0 ! Aerosol Sedimentation
IALEAK 0 ! Aerosol Leakage
IFOG 0 ! Fog formation
ISRC 1 ! User-defined sources
IMCO 0 ! MCO models
ISENS 0 ! Sensitivity runs
END ACTIVE MODELS ! ACTIVE MODELS is a comment

C-----
C SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
C
C END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS

FAI/98-40, Rev. 1

Date: 12/31/98

A - 2

FAI/98-40, Rev. 1

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GASES      1      2      3
STEAM      1.00  1.00  1.00
NITROGEN   1.0e-6 1.0e-6 1.0e-6
END GASES  ! GASES is a comment
END VOLUMES ! VOLUMES is a comment

DACO 0 ! MCO models
ISENS 0 ! Sensitivity runs
END ACTIVE MODELS ! ACTIVE MODELS is a comment
END CONTROL ! End of CONTROL keyword group

```

A.2 Fog Formation Validation Test

```

CONTROL ! Major keyword group

TITLE ! Keyword; next line is title, title can be any length
Fog Formation Validation Test
END TITLE ! Anything after END is a comment

TIMING ! Keyword
TSTART 0 ! START TIME, >0 FOR RESTART RUN
! RESTART FILE IS READ FROM HANSEF.RER
! END TIME (Seconds)
TLAST 0.80
DTMIN 0.0 0.10 ! MIN TIMESTEP (Seconds)
DTMAX 0.0 0.10 ! MAX TIMESTEP (Seconds)
DTPRIN 0.0 0.1 ! PRINT INTERVAL (Seconds)
PLTMIN 0.0 0.10 ! MIN PLOT INTERVAL WITHOUT PLOT (Seconds)
PLTMAX 0.0 0.10 ! MAX PLOT INTERVAL WITHOUT PLOT (Seconds)
DTTEST 0.0 0.8 ! RESTART INTERVAL (Seconds)
FTFCH 0.005 ! FRACTIONAL CHANGE IN T AND P
FAECH 0.005 ! FRACTIONAL CHANGE IN AEROSOL MASS
FPPLCH 0.03 ! FRACTIONAL CHANGE FOR PLOTTING
END TIMING ! TIMING is a comment.

```

```

ACTIVE MODELS ! Keyword; MODELS is a comment; 1 = on, 0 = off
IUNC 0 ! Junction flow model
ICCFLOW 0 ! Counter-current flow model
INSNK 0 ! Heat sinks
ICNDS 0 ! Condensation
IASED 0 ! Aerosol Sedimentation
IALEAK 0 ! Aerosol Leakage
IFOG 1 ! Fog formation
ISRC 0 ! User-defined sources

```

FAI/98-40, Rev. 1

A - 3

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VOLUMES 2 ! total number of control volumes
* VOLUME m^3, SED_AREA m^2, ELEVATION m, TEMP_GAS C, PRESSURE Pa
*
REGIONS 1 2
VOLUME 1.000 1.000
SED_AREA 0.000 0.000
ELEVATION 0.000 0.000
TEMP_GAS 50.00 50.00
PRESSURE 1.000E5 1.000E5
END REGIONS ! REGIONS is a comment
*
GASES 1 2
STEAM 0.15 0.00
METHANOL 0.00 0.40
NITROGEN 0.85 0.60
END GASES ! GASES is a comment
END VOLUMES ! VOLUMES is a comment

```

A.3 Inter-Compartmental Flow Validation Test

```

CONTROL ! Major keyword group
*
*
TITLE ! Keyword; next line is title, title can be any length
Flow and Thermodynamic Validation Test
END TITLE ! Anything after END is a comment
*
*
TIMING ! Keyword
TSTART 0
TLAST 1002.0
DTPRIN 0.0 1.00
DTMAX 0.0 1.00
DTPRIN 0.0 100.0
END TIMING ! TIMING is a comment
*
START TIME, >0 FOR RESTART RUN
RESTART FILE IS READ FROM HANSEF.RER
END TIME (Seconds)
MIN TIMESTEP (Seconds)
MAX TIMESTEP (Seconds)
PRINT INTERVAL (Seconds)

```

Date: 12/31/98

Date: 12/31/98

A - 4

FAI/98-40, Rev. 1

```

PRESSURE 1.000E5 1.000E5
END REGIONS ! REGIONS is a comment
*
GASES 1 2
STEAM 0.01 0.01
NITROGEN 0.79 0.79
OXYGEN 0.20 0.20
END GASES ! GASES is a comment
END VOLUMES ! VOLUMES is a comment
JUNCTIONS 1
PATHS 1
IUTYP 1
IRI 1
IR2 2
IUGRIZ 1
KXJN 0.20
XLJN 0.01
AJN 0.03
ZJN 5.0
ZJN 10.0
CJN 3.5
CJN 0
END PATHS
END JUNCTIONS

```

A.4 Heat Transfer Model Validation Test

```

CONTROL
TITLE Heat Transfer Model Validation Test
END TITLE
TIMING
TSTART 0.0 ! START TIME, >0 FOR RESTART RUN
! RESTART FILE IS READ FROM HANSF.REW
! END TIMESTEP
! MAX TIMESTEP
! PRINT INTERVAL
! MIN PLOT INTERVAL
! MAX PLOT INTERVAL WITHOUT PLOT
! RESTART INTERVAL
! RESTART IS WRITTEN TO HANSF.REW
DTRST 250000.0

```

```

PLTMIN 0.0 5.0 ! MIN PLOT INTERVAL (Seconds)
PLTMAX 0.0 5.0 ! MAX INTERVAL WITHOUT PLOT (Seconds)
DTRST 0.0 100000. ! RESTART INTERVAL (Seconds)
PFCH 0.005 ! FRACTIONAL CHANGE IN T AND P
PFCH 0.005 ! FRACTIONAL CHANGE IN AEROSOL MASS
PFCH 0.03 ! FRACTIONAL CHANGE FOR PLOTTING
END TIMING ! TIMING is a comment.
*
ACTIVE MODELS ! Keyword; MODELS is a comment; 1 = on, 0 = off
IJUNC 1 ! Junction flow model
IHSINK 0 ! Counter-current flow model
ICNDNS 0 ! Condensation
IASED 1 ! Aerosol Sedimentation
IAERAK 0 ! Aerosol Package
IFGC 1 ! Particle Formation
IMCO 0 ! User-defined sources
ISNS 0 ! MCO models
END ACTIVE MODELS ! ACTIVE MODELS is a comment
*
C-----
C SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
C END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
C ENTER: TIME, TEMP, FLOWRATES, POWER
C SYNTAX EXAMPLE:
C SOURCES 1 ! -- KEYWORD AND # SOURCE GROUPS
C REGION 1 GASES 2 ! -- REGION # AND # GASES
C STEAM CARBON DIO ! -- GAS NAMES MUST BE ON NEXT LINE
C 0.0 1726.85 0.5 0.5 0.0
C 100.0 1726.85 0.5 0.5 0.0
C 1.0 26.85 0.0 0.0 0.0
C 1.85 26.85 0.0 0.0 0.0
C END REGION ! -- ENDS A REGION SOURCE
C END SOURCE ! -- ENDS ALL SOURCE INPUT
*
PLOT
GAS-T 1 1
PRESSURE 1 1
END PLOT
*
END CONTROL ! End of CONTROL keyword group
*
VOLUMES 2 ! Total number of control volumes
* VOLUME m^3, SED_AREA m^2, ELEVATION m, TEMP GAS C, PRESSURE Pa
*
REGIONS 1 2
VOLUME 850.0 1.E10
SED_AREA 88.2 0.000
ELEVATION 0.000
TEMP_GAS 26.85

```

Date: 12/31/98

```

IREGI 1 1 Region index for inside surface
I=0 for insulated, -1 for constant temperature
TIHS 0.0 1 constant temperature for IREGI = -1
INREG 0 1 Region index for outside surface
I=0 for insulated, -1 for constant temperature
TOHS 0.0 1 constant temperature for IREGI = -1
EHSI 0.7 1 emissivity of inside surface
EHSO 0.7 1 emissivity of outside surface
END HEAT_SINKS
END HEAT_SINKS

```

A.5 Aerosol Experiment Validation

CONTROL

```

TITLE
Aerosol Leakage Model Validation Test
END TITLE

```

```

TIMING
TSTART 0.0 1 START TIME, >0 FOR RESTART RUN
1 RESTART FILE IS READ FROM HANSF.REW
TLAST 5.0 1 END TIME
DTMIN 0.01 1 MIN TIMESTEP
DTMAX 0.01 1 MAX TIMESTEP
DTRIN 0.5 1 PRINT INTERVAL
PLTMIN 0.5 1 MIN PLOT INTERVAL
PLTMAX 0.5 1 MAX INTERVAL WITHOUT PLOT
DTRST 501.0 1 RESTART INTERVAL
1 RESTART IS WRITTEN TO HANSF.REW
1 RESTART IS WRITTEN IN T AND P
FTFCH 0.005 1 FRACTIONAL CHANGE IN T AND P
FPFLCH 0.03 1 FRACTIONAL CHANGE FOR PLOTTING
END TIMING

```

ACTIVE MODELS

```

1JUNC 1 1 Use junction model
1CFILW 1 1 Use junction counter-current flow model
1HSINK 0 1 Use heat sink model
1CNDS 0 1 Use condensation model
1TASD 0 1 Use aerosol sedimentation model
1TASX 1 1 Use aerosol flow between compartments
1FOG 0 1 Use fog formation/evaporation models
1SRC 0 1 Use source models
1ISNS 0 1 Use MCO models
1ISNS 0 1 Use MCO models
END ACTIVE MODELS

```

```

PLOT
PRESSURE 1 1
GAS-T 1 1
AER-PASS CSOR 2 1 2
END PLOT

```

```

0.005 1 FRACTIONAL CHANGE IN T AND P
0.03 1 FRACTIONAL CHANGE FOR PLOTTING

```

END TIMING

ACTIVE MODELS

```

1JUNC 0 1 Use junction model
1CFILW 0 1 Use junction counter-current flow model
1HSINK 0 1 Use heat sink model
1CNDS 0 1 Use condensation model
1TASD 0 1 Use aerosol sedimentation model
1TASX 0 1 Use aerosol flow between compartments
1FOG 0 1 Use fog formation/evaporation models
1SRC 0 1 Use source models
1ISNS 0 1 Use MCO models
1ISNS 0 1 Use MCO models
END ACTIVE MODELS

```

PLOT

```

HS-TI 1 1
HS-TO 1 1
END PLOT

```

END CONTROL

VOLUMES 1

```

REGIONS
VOLUME 1 1.010
ELEVATION 0.0
TEMP GAS 100.00
PRESSURE 1.05
END REGIONS

```

END REGIONS

GASES

```

NITROGEN 1
OXYGEN 0.8
END GASES

```

END GASES

END VOLUMES

HEAT SINKS 1

```

1 1
1GEOM 1 1 Use plane wall, 2=Cylindrical
RHO 500.0 1 density
KHS 500.0 1 thermal conductivity
KHS 500.0 1 specific heat
KHS 500.0 1 volumetric heat generation
KHS 500.0 1 inner radius
KHS 500.0 1 outer radius; outer-inner-thickness for plane
KHS 500.0 1 area
KHS 100.0 1 characteristic length for natural convection
KHS 10.0 1 initial inside surface temperature
KHS 200.0 1 initial outside surface temperature (linear)
KHS 200.0 1 number of slabs (min. 3)
KHS 10 1
END HEAT SINKS

```

END HEAT SINKS

END HEAT SINKS

END HEAT SINKS

END HEAT SINKS

END HEAT SINKS

END HEAT SINKS


```

END CONTROL
VOLUMES 2
  REGIONS
  VOLUME 1 2
  SED_AREA 1.04 1.0
  RESTART 0.0 0.0
  TEMP 26.85
  PRESSURE 1.2e5
  END REGIONS
  GASES 1 2
  NITROGEN 1.0 1.0
  END GASES
  AEROSOLS 1 2
  CSOH 0.001 0.0
  END AEROSOLS
  END VOLUMES
  JUNCTIONS 1
  PATHS 1
  IUTYP 1
  IR2 1
  IHORIZ 1
  IR2 1
  IHORIZ 1
  XNHN 0.11
  XNHN 0.11
  XLJN 0.01
  XLJN 0.01
  ZJN 5.0
  ZJN 10.0
  CUN 1.5
  CUN 1.0
  N90 0
  END PATHS
  END JUNCTIONS
  TITLE
  COUNTER-CURRENT FLOW MODEL VALIDATION, CASE-1
  END TITLE
  TIMING
  TSTART 0.0
  TLAST 3600.0
  TMIN 0.1
  DMAX 1.0
  DPRINT 100.0
  ! START TIME, >0 FOR RESTART RUN
  ! RESTART FILE IS READ FROM HANSF.RER
  ! END TIME
  ! MIN TIMESTEP
  ! MAX TIMESTEP
  ! PRINT INTERVAL
  ! MIN PLOT INTERVAL
  ! MAX INTERVAL WITHOUT PLOT
  ! RESTART IS WRITTEN TO HANSF.REW
  ! FRACTIONAL CHANGE IN T AND P
  ! FRACTIONAL CHANGE FOR PLOTTING
  !
  PLOTMIN 1.0
  PLOTMAX 10.0
  DTRST 3600.
  FTFCH 0.005
  FPFCH 0.03
  END
  ACTIVE MODELS
  IOUNC 1
  IOUNC 1
  IOUNC 1
  IHSTNK 0
  ICNGS 0
  IASED 0
  IALEAK 0
  IFOG 0
  ISRC 0
  IMCO 0
  ISNS 0
  END
  PLOT
  PRESSURE 1 1
  GAS-T 2 1
  GAS-X STEAM 2 1
  GAS-W 1 1
  GAS-WX 1 1
  END
  END VOLUMES 2
  REGIONS 1 2
  VOLUME 100.0 100.0
  SED_AREA 21.4 21.4
  ELEVATION 4.63 0.0
  TEMP GAS 20.00 1.0135
  PRESSURE 1.0135 1.0135
  END REGIONS 1 2
  GASES 1 2
  NITROGEN 0.790 0.790
  OXYGEN 0.200 0.200
  STEAM 0.010 0.010
  END GASES
  END VOLUMES
  JUNCTIONS 1
  PATHS 1
  IUTYP 1
  IHORIZ 1
  IR2 1
  IR2 2
  IHORIZ 1
  XNHN 1.9
  XNHN 2.1
  XLJN 0.5
  XLJN 0.5
  ZJN 0.
  ZJN 4.63
  CUN 1.
  CUN 1.0
  N90 1.0
  
```

A.6 Counter-Current Flow Model Validation

```

CONTROL
TITLE
COUNTER-CURRENT FLOW MODEL VALIDATION, CASE-1
END TITLE
TIMING
TSTART 0.0
TLAST 3600.0
TMIN 0.1
DMAX 1.0
DPRINT 100.0
! START TIME, >0 FOR RESTART RUN
! RESTART FILE IS READ FROM HANSF.RER
! END TIME
! MIN TIMESTEP
! MAX TIMESTEP
! PRINT INTERVAL

```

end of the input deck

CONTROL

```

TIMING
! START TIME, >0 FOR RESTART RUN
! RESTART FILE IS READ FROM HANSF.REW
!
! MIN TIME
! MAX TIME
! MIN TIMESTEP
! MAX TIMESTEP
! PRINT INTERVAL
!
! MIN PLOT INTERVAL
! MAX INTERVAL WITHOUT PLOT
! RESTART INTERVAL
! RESTART IS WRITTEN TO HANSF.REW
!
! FRACTIONAL CHANGE IN T AND P
! FRACTIONAL CHANGE FOR PLOTTING
!
! FPELCH
!
END TIMING
0.0
0.25
0.001
0.001
0.001
0.001
0.010
0.010
501.0
0.005
0.03

```

IUNFC	1	1-Use function model
IUNFLW	0	1-Use function counter-current flow model
ICESHL	0	1-Use heat sink model
ISHSNK	0	1-Use condensation model
ICNDS	0	1-Use aerosol sedimentation model
IASESD	0	1-Use aerosol compartment models
IAPLEAK	1	1-Use fog fraction/evaporation models
IFOG	0	1-Use fog fraction models
ISRC	0	1-Use MCO models
IMCO	0	1-
ISNSK	0	1-

```

TITLE          ! Keyword; next line is title, title can be any length
EVAPORATION VALIDATION
END TITLE      ! Anything after END is a comment
TIMING         ! Keyword

```

A.8 Evaporation/Condensation Validation

***** EVAPOR.DAT *****

UNIT ESS OTHERWISE NOTED, MKS UNITS

number 1 major keyword group

TITLE ! Keyword; next line is title, title can be any length
EVAPORATION VALIDATION
END ! Everything after END is a comment

TIMING | **Keyword**

FAI/98-40, Rev. 1

```

      STEPM          0.0           0.0
    END AEROSOLS ! AEROSOLS is a comment

**
** OPTIONAL TEMPERATURE AND PRESSURE CONTROL
** CONTROL MCO HEATUP GASES AND INLET GAS TEMPERATURE
** CONTROL MCO HEATUP GASES AND INLET GAS TEMPERATURE
** IMPOSE TEMPERATURE LOOK-UP TABLE
** SYNTAX:
**   EXTRAPOLATION_TIMETG
**   TIMEG IRSG TIME1, TIME2...TIMELAST
**   PREFIX IRSG TEMP1, TEMP2...TEMPLAST
**   LINEAR INTERPOLATION BETWEEN VALUES
**
** SIMILAR SYNTAX FOR PRESSURE:
**   OFFSET TIMETG
**   EXTRAPOLATION_TIMETG
**   TIMEP IRPG TIME1, TIME2...PRESSURES ARE IN PA!!!
**   PREFIX IRPG PRES1, PRES2...PRESSURES ARE IN PA!!!
**
** OFFSET_TIMETG= OFFSET TIME; ENTER LOOKUP TABLE WITH
**                  TIME+OFFSET_TIMETG
**   EXTRAPOLATION_TIMETG= LAST TO USE LAST VALUE IN THE TABLE,
**                        = ENTROPY TO EXTRAPOLATE FROM LAST TWO POINTS,
**                        = PERIOD TO WRAP AROUND.
**
**   OFFSET TIMETG          50 LAST
**   EXTRAPOLATION_TIMETG  200
**   TIMEG 1 293.15 373.15 473.15
**   TGPX 1 293.15 373.15 473.15
**
** CONTROL MCO BOUNDARY P, 30, ENTHRAP
**   OFFSET TIMEFG
**   EXTRAPOLATION_TIMEFG
**   TIMEP 1 0.0 10.0 200
**   PREFIX 1 1.E5 1.2E5 1.4E5
**
** END VOLUMES ! VOLUMES is a comment
END VOLUMES

**
** Major keyword----- Total number of heat sinks
HEAT_SINKS 15 -----
** decay power based on 835 W per MCO.
** No more than 5 columns at a time,
** Select the following structure,
** SINKS
**
**
**
**
**
**
** Syntax:
** 1 for plane, 0 or 2 for cylinder
** RHO Density (kg/m^3)
** KHS Thermal Conductivity (W/m/K)
** CPHS Specific Heat (J/kg/K)
** QV Volumetric Heat Generation (W/m^3)
** XRI Inner Radius (m); for plane wall, thickness = XRO-XRI
** XRO Outer radius (m); for sphere, thickness = XRO-XRI
** XRO provided heat sink area (m^2)

```

```

* SINKS 11 12 13 14 15
* IGBOM 18768.1 18768.1 18768.1
* RHO 26.9 26.9 26.9
* KHS 122.67 122.67 122.67
* CPHS 0.00 0.00 0.00
* QV 0.0 0.0 0.0
* QV1 0.0 0.0 0.0
* XRO 0.00698 0.00783 0.00698
* AHS 1.310 1.310 1.310
* TIMIN 75.0 75.0 75.0
* TOINLT 75.0 75.0 75.0
* IMSLAB 3 3 3
* IREGI 0.0 0.0 0.0
* TIRS 1 1 1
* IREGO 0.0 0.0 0.0
* XHS 0.661 0.663 0.663
* EHSI 0.7 0.7 0.7
* EHSO 0.7 0.7 0.7
* END

* USER CAN CONTROL HEAT SINK BOUNDARY TEMPERATURE
* SYNTAX:
* EXTRAPOLATION TIMERS
* TIMSIX IHS ISD TIME1, TIME2...
* TIMSIX IHS ISD TIME1, TIME2...
* IHS = HEAT SINK NO. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15
* CONTROL HEAT SINK BOUNDARY T.
* EXTRAP
* TIMSIX 15 2 0.0 1.66
* TIMSIX 15 2 75.0 75.0
* TIMSIX 30 2 0.0 1.66
* TIMSIX 30 2 75.0 75.0
* TIMSIX 41 2 0.0 1.66
* TIMSIX 41 2 75.0 75.0
* TIMSIX 42 1 0.0 1.66
* TIMSIX 42 1 75.0 75.0
* TIMSIX 42 2 0.0 1.66
* TIMSIX 42 2 75.0 75.0
* END HEAT SINKS ! HEAT SINKS is a comment
* JUNCTIONS 0 1 0 Junctions
* Syntax:
* LUTYP Junction Type: 1 = Normal, 2 = HEPA, 3 = Cover
* IR1 Upstream Region
* IR2 Downstream Region
* AIN Area (m^2) for HEPA Junction (m^2)
* AINP Area (m^2) for HEPA Filter Failure Pressure (Pa)
* ACOV Cover Area (m^2)
* MCOV Cover Weight (kg)

```

A - 10

```

XGPCSK 0.0155 ! gap distance between the MCO wall and the cask
FITLID 0.0 ! =0, turn off the radiative heat transfer between the
! =1, fully account for the radiative heat transfer
RHOSL 5000. ! sludge specific heat (Btu/m^3)
XSL 1000. ! sludge particle area (m^2/m^3)
XDSL 1.E-6 ! sludge particle diameter (m)

* Hydrate Model: two-step decomposition,
* input curves for IN P and IN K
* first step for x > XHYD2, second step for x < XHYD2
*
* 10 weight fraction of sludge being water is equivalent to 90 %
* of sludge being hydrated with 2 moles of
* water per mole of uranium oxide
*
* FVSL 0.9 ! fraction of sludge that is hydrated
* XVSL 2.0 ! stoichiometry number of hydrate; no. of moles of
! water per mole of uranium oxide (UO3.H2O)
*
* XHYD2 1.0 ! H2O/U ratio (stoich. number) to switch
! from first to second dehydration law
*
* XHYD3 0.5 ! H2O/U ratio to third correlation
!
* AHYE01 18.012 ! 'A' IN LN P = A + B/T FOR X > XHYD2
* BHYE01 -6775.E0 ! 'B' IN LN P = A + B/T FOR X > XHYD2
* AHYE02 19.076 ! 'A' IN LN P = A + B/T FOR X < XHYD2
* BHYE02 -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD2
* AHYE03 19.076 ! 'A' IN LN P = A + B/T FOR X < XHYD3
* BHYE03 -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD3
* ADEH1 -5.425E0 ! 'A' IN LN K = A + B/T FOR X > XHYD2
* BDEH1 -5.425E0 ! 'B' IN LN K = A + B/T FOR X > XHYD2
* ADEH2 -5.295E0 ! 'A' IN LN K = A + B/T FOR X < XHYD2
* BDEH2 -5.295E0 ! 'B' IN LN K = A + B/T FOR X < XHYD2
* ADEH3 -2546.E0 ! 'A' IN LN K = A + B/T FOR X < XHYD3
* BDEH3 -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD3
* DHX1 2.8686 ! Decomposition enthalpy J/Kg H2O: 1st step
* DHX2 3.7086 ! Decomposition enthalpy J/Kg H2O: 2nd step
* DHX3 4.7086 ! Decomposition enthalpy J/Kg H2O: 3rd step
* FCONHY 1.0 ! hydride production rate law multiplier
* FCONHY 1.0 ! hydride consumption rate law multiplier
* ENTRI 1.0 ! nitriding rate law multiplier

* PUMP, FEED, AND CONDENSER MODELS
* Syntax:
* PUMP IRPUM IROPM ICONPM ITFED WUPUMP WUFED TGFED TCONPM
* Definitions:
* IRPUM - Pump inlet region
* IROPM - Pump outlet region
* ICONPM - Node to which the condensed steam is dumped for book-keeping
* ITFED - If non-zero, overrides TGFED with the designated region
* temperature. Used to specified time-varying feed
* temperature
* WUPUMP - Feed volumetric flowrate (m^3/s)
* WUFED - Feed volumetric flowrate (m^3/s)
* TCONPM - Feed temperature (K)
* FCONPM - Condenser cooling coil temperature (K)
* 35 FT^3/MIN * 1 MIN/60 SEC * 0.02832 M^3/1 FT^3 = 0.01652 M^3/SEC

```

```

* PUMP IRPUM IROPM ICONPM ITFED WUPUMP WUFED TGFED TCONPM
* PUMP 1 5 0 0 1.652E-2 0.0 0.0 0.0
* Radiolysis parameters
*
* FRAD 1.0 ! multiplier for radiolysis
* FALPHA 0.197 ! alpha fractional heat load
* FBETA 0.486 ! beta fractional heat load
* FGAMMA 0.317 ! gamma fractional heat load
* QHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
! of water
* FGEN 1.0 ! general isotope loading
* FGENERAL 1 ! GENERAL is a comment
*
* END GENERAL
*
* SOLAR_RAD
*
* pointers to heat sinks representing the cask wall and the top
* solar radiation impinges on these
*
* IHCSK 42
* IHOP 44
*
* look-up table for solar radiation throughout a day (sec. vs. W/m^2)
*
* OFFSET_TMDAY 21600. ! offset by six hours
* EXTRAPOLATION_TMDAY PERIOD ! repeat the diurnal cycle
* TMDAY 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
* 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
* 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
* 75600.0 79200.0 82800.0 86400.0
*
* RADSN 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
*
* END SOLAR_RAD
*
* FUEL_BSNT 1 ! Total number of fuel baskets
*
* 1st Fuel Basket
*
* IHSPFL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
*
* define the heat sinks comprising the first fuel basket (must be
* in pairs, for inner and outer elements)
*
* IFLINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
* IFLMCO 15 ! define the adjacent MCO wall heat sink
* IFLAID 0 ! define the lid or floor heat sink to which the fuel
! radiate to
* AFLFL 0.131 ! flow area in the basket
*
* fraction of geometric area exposed for oxidation
* = area available for oxidation/total heat sink area
*
* FNOXFL 0.036 0.036 0.036 0.036 0.036 0.036 0.036 0.036
* 0.036 0.036 0.036 0.036 0.036 0.036
* FOX 0.036 0.0 ! multiplier for FAOXFL
* XFLOXO 0.01 ! initial oxide (oxide-hydride) thickness (to be
! applied to
! exposed area)

```

A.9A Hydride Decomposition Validation

```

*****
* HYDRADE DECOMPOSITION VALIDATION: HYDDEC.DAT
*
* UNLESS OTHERWISE NOTED, MKS UNITS
*
* - 1 TIER OF SCRAP BASKET
* - 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
*
*****
*
* CONTROL ! Major keyword group
*****

```

Date: 12/31/98

A - 13

FAI/98-40, Rev. 1

```

*-----*
*
* TITLE      : Keyword; next line is title, title can be any length
* HINDS FORMATION VALIDATION
* END TITLE : Anything after END is a comment
*
*-----*
*
* TTMING      : Keyword
*
* TSTART      :
* 200.
* 0.001
* 1. 20.
* 10.
* 100.
* 250.
* 0.005
* 0.005
* 0.03
* END TIMING : TIMING is a comment.
*
* PLOT        : Keyword for plotting section
* Plotting syntax:
* PRESSURE n rlist - Gas Temperature, Pa
* GAS-T n rlist - Gas Temperature, K
* HS-TI n rlist - Heat Sink Temperature - Inner Surface, K
* HS-TO n rlist - Heat Sink Temperature - Outer Surface, K
* HS-T n rlist - Heat Sink Temperature - Average, K
* AEROSOL n rlist - Aerosol Mass (Total), kg
* GAS-W n rlist - Mass Flowrate, kg/s
* GAS-WX n rlist - Counter-Current Mass Flowrate, kg/s
* GAS-X GASNAME n rlist - Gas Mole Fraction
* GAS-RH GASNAME n rlist - Gas Relative Humidity
* GAS-MASS GASNAME n rlist - Gas Mass (Species), kg
* AER-MASS GASNAME n rlist - Aerosol Mass (Species), kg
* MASS GASNAME n rlist - Total Mass (Species), kg
* LIQ-MASS - GASNAME n rlist - Deposited Mass (Species), kg
*
* Pressure, Gas Temperature, and total aerosol mass require a region
* list
*
* Heat sink temperatures need a heat sink number list
*
* Flowrates need a junction number list
*
* Gas concentration, relative humidity, individual species gas mass,
* individual species aerosol mass, total (gas+aerosol) individual
* species mass, and individual species deposited liquid mass require
* a region and gas name
*
* END PLOT : PLOT is a comment
*
* ACTIVE MODELS : Keyword; MODELS is a comment; 1 = on, 0 = off
* IJUNC 0 : Junction flow model
*
*-----*
*
* ICCELW 0 : Counter-current flow model
* IHSINK 1 : Heat sinks
* CONDENS 0 : Condensation
* IASED 0 : Aerosol Sedimentation
* IALEAK 0 : Aerosol Leakage
* IFOG 0 : Fog Deposition
* IUC 0 : User-defined sources
* IMCO 1 : MCO models
* ISENS 0 : Sensitivity runs
*
* END ACTIVE MODELS : ACTIVE MODELS is a comment
*
*-----*
*
* SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
* ENTER: TIME, TEMP, FLOWRATES, POWER
*
* SYNTAX EXAMPLE:
* SOURCES 2 1 -- KEYWORD AND # SOURCE GROUPS
* REGION 1 1 -- REGION #, # GASES
* STREAM HYDROGEN 1 -- GAS NAMES MUST BE ON NEXT LINE
* 0 300 1.E-3 1.E-3 0.E0
* 10 300 1.E-3 1.E-3 0.E0
*
* END REGION 1 -- ENDS A REGION SOURCE
* REGION -1 GASES 1 1 -- FOR AEROSOL, SPECIFY -IVE REGION
* NA2O
* 0. 300.0 4.44E-1 0.E0
* 10. 300.0 4.44E-1 0.E0
* 900. 300.0 4.44E-1 0.E0
* 901. 300.0 0.E0 0.E0
* 1.E5 300.0 0.E0 0.E0
*
* END SOURCE
*
* END CONTROL : End of control keyword group
*
*-----*
*
* VOLUMES 1 : total number of control volumes
*
* REGIONS
* VOLUME 1-0
* SED AREA 0.0
* ELEVATION 0.0
* TEMP GAS 299.85
* PRESSURE 1.E5
*
* END REGIONS
*
* Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
*
* GASES
* HELIUM 1
* ARGON 0.99
* END GASES
*
* Aerosol concentration of each region (kg/m^3)

```


A - 14

A - 15

IHSCSK 15 ! define the cask heat sink
 IRGAP 1 ! define the gap node (between MCO wall and the cask)
 ! radiative/conductive h.t. between the MCO wall and
 ! the cask is computed and some of the heat is
 diverted
 XPGCEK 0.0155 ! to gas for stability (the MCO wall and the cask
 FHTLID 0.0 ! gap distance between the MCO wall and the cask
 ! -0, turn off the radiative heat transfer between the
 ! fully accreted lid/floor
 ! -1, fully accreted lid for radiative heat transfer
 RHOSL 5000. ! sludge particle density (kg/m³)
 SASL 1000. ! sludge specific area (m²/m³)
 XDSL 1.E-6 ! sludge particle diameter (m)
 * Hydrate Model, two-step decomposition,
 * input areas for ln P and ln K
 * first step for x > XHYD2, second step for x < XHYD2
 * 10 & weight fraction of sludge being water is equivalent to 90 %
 * of water being hydrated with 2 moles of
 * water per mole of uranium oxide
 FHYSL 0.9 ! fraction of sludge that is hydrated
 XHYSL 2.0 ! stoichiometry number of hydrate; no. of moles of
 ! H₂O per mole of uranium oxide (H₂O:H₂O)
 XHYD2 1.0 ! H₂O/U ratio (stoich. number) to switch
 ! from first to second correlation
 XHYD3 0.5 ! H₂O/U ratio (stoich. number) to switch
 ! from second to third correlation
 AHYEQ1 18.012 ! 'A' in ln P = A + B/T FOR X > XHYD2
 BHVEQ1 -6775.E0 ! 'B' in ln P = A + B/T FOR X > XHYD2
 AHYEQ2 19.076 ! 'A' in ln P = A + B/T FOR X < XHYD2
 BHVEQ2 -8312.E0 ! 'B' in ln P = A + B/T FOR X < XHYD2
 AHYEQ3 19.076 ! 'A' in ln P = A + B/T FOR X < XHYD3
 BHVEQ3 -8312.E0 ! 'B' in ln P = A + B/T FOR X < XHYD3
 ADHY1 -5.4395E0 ! 'A' in ln K = A + B/T FOR X > XHYD2
 BDHY1 -2.5495E0 ! 'B' in ln K = A + B/T FOR X > XHYD2
 ADHY2 -2.5495E0 ! 'A' in ln K = A + B/T FOR X < XHYD2
 BDHY2 -2546.E0 ! 'B' in ln K = A + B/T FOR X < XHYD2
 ADHY3 -5.495E0 ! 'A' in ln K = A + B/T FOR X < XHYD3
 BDHY3 -2546.E0 ! 'B' in ln K = A + B/T FOR X < XHYD3
 DHY1 2.86E6 ! Decomposition enthalpy J/kg H₂O: 1st step
 DHY2 3.70E6 ! Decomposition enthalpy J/kg H₂O: 2nd step
 DHY3 3.70E6 ! Decomposition enthalpy J/kg H₂O: 3rd step
 FPROH 1.0 ! hydrate production rate law multiplier
 FCONHY 1.0 ! hydrate consumption rate law multiplier
 FNTRI 1.0 ! nitriding rate law multiplier
 * PUMP, FEED, AND CONDENSER MODELS
 SYNTAX !
 PUMP IRUPUM IRUPUM ITCNPM ITFEED WVPUMP WVFEEED TCONCPM
 * Definitions:
 IRUPUM - Pump inlet region
 IRUPUM - Pump outlet region
 ITCNPM - Node to which the condensed steam is dumped for book-keeping
 ITCNPM - If non-zero, overrides TGFEEED with the designated region
 ITFEED - Temperature. Used to specified time-varying feed
 temperature

A - 16

FAI/98-40, Rev. 1

WVPUMP - Pump volumetric flowrate (m³/s)
 WVFEEED - Feed volumetric flowrate (m³/s)
 TGFEEED - Feed temperature (K)
 TCONCPM - Condenser cooling coil temperature (K)
 * 35 FT³/MIN * 1 MIN/60 SEC * 0.02832 M³/1 FT³ = 0.01652 M³/SEC
 WVPUMP WVFEEED TGFEEED TCONCPM
 PUMP 1 5 0 0 1.652E-2 0.0 0.0 0.0
 * Radiolysis parameters
 FRAD 1.0 ! multiplier for radiolysis
 FALPHA 0.197 ! alpha fractional heat load
 FBETA 0.486 ! beta fractional heat load
 FGAMMA 0.317 ! gamma fractional heat load
 QPHOTO 2.4E-6 ! heat deposition rate in MCO from water per gram
 ! per MTU of fuel loading
 ! GENERAL is a comment
 END GENERAL
 * SOLAR_RAD
 * pointers to heat sinks representing the cask wall and the top
 * solar radiation impinges on these
 * IHCSK 42
 * IHTOP 44
 * look-up table for solar radiation throughout a day (sec vs. W/m²)
 * 21600. ! offset by six hours
 * OFFSET TIMDAY PERIOD ! repeat the diurnal cycle
 * EXTRAPOLATION TIMDAY PERIOD ! repeat the diurnal cycle
 * TIMDAY 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
 * 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
 * 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
 * 75600.0 79200.0 82800.0 86400.0
 * RAD SUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * END SOLAR_RAD
 * FUEL_BSNT 1 ! Total number of fuel baskets
 * 1st Fuel Basket
 * INSFL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
 * ! define the heat sinks comprising the first fuel basket (must be
 * ! in pairs, for inner and outer elements)
 * ! define the adjacent center insert heat sink,
 * ! 0 for no insert
 * IFLINS 0
 * ! define the adjacent MCO wall heat sink
 * IFLMCO 15
 * ! define the lid or floor heat sink to which the fuel
 * ! radiates to
 * IFLID 0
 * ! flow area in the basket
 * AFLEL 0.131
 * ! fraction of geometric area exposed for oxidation
 * ! = area available for oxidation/total heat sink area

```

* ISCMCO 41 ! define the adjacent MCO wall heat sink
* ISCLID 44 ! define the lid or floor heat sink to which the
scrap
! rediate to
* proximity of the scrap for each heat sink in the order read in
(31, 32, 33, 34, ..)
* PROPOS 0.45 0.45 0.45 0.45 0.45 0.6 0.6 0.6 0.6
* characteristic size for each scrap heat sink in the order read in (m)
* XDSCR 0.00635 0.00635 0.00635 0.00635 0.00635
* XRSBCK 0.2860 ! radius of scrap basket (m)
* XRSBCK 0.691 ! height of scrap basket (m)
* exposed surface area available for oxidation
per unit volume of scrap (1/m) for
each scrap basket heat sink in the order read in
* XSCXCO 0.0 ! initial oxide thickness on the exposed surface (m)
* XSCXCO 0.0 ! initial oxide thickness on the exposed surface (m)
* AVONSC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
* FOXSC 10.0 ! multiplier for AVONSC
* XSCXCO 0.0 ! initial oxide thickness on the exposed surface (m)
* ESCHVD 0.0 ! fraction of oxide which is hydrate
* 1.5 kg of water total for scrap basket; 1.5/0.17491 8.576 kg/m3
* MVNSCO 8.576 ! initial amount (kg) of water per unit bulk volume
* MVNSCO 0.0 ! (m3) of scrap surface of the insert
! on the outer surface of the MCO wall
* FMSCIO 0.0 ! (per unit area, m2)
! on the inner surface of the MCO wall
* FMSCH0 0.0 ! (per unit area, m2)
! wetted fraction of surface area
* FMSCH 0.1 ! wetted fraction of MCO wall
* FMSCH 1.0 ! gap distance between the insert and scrap basket
* XSCMCO 0.00635 ! gap distance between the insert and MCO wall
* MSISC 55.0 ! mass of sludge particles (kg) in the scrap basket
* END IHSCF for 1st scrap basket
* END SCRAP_BSKT
* END MCO

```

A.9B Hydride Formation Validation

```

*****
HYDRIDE FORMATION VALIDATION: HYDRO.DNT
UNLESS OTHERWISE NOTED, MKS UNITS
- 1 TIERS OF SCRAP BASKET
- 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
*****

```

A - 17

```

* FMOXEL 0.036 0.036 0.036 0.036 0.036 0.036 0.036 0.036
* FOX 0.036 0.036 0.036 0.036 0.036 0.036 0.036 0.036
* FOXO 0.01 ! initial oxide (oxidohydride) thickness (to be
applied to
* EXHVD 1.0 ! exposed area)
* fraction of initial oxide which is hydrate
* initial amount (kg) of water per geometric surface area (m2) of fuel
(2433.6 m2) = 0.3571
* 8.472/16.8 = 0.256 kg/m2 (per side)
* FFWLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* FFWLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* FFWLO 0.0 ! on the outer surface of the insert
* FFWLO 0.0 ! on the outer surface of the MCO wall
* FFWLO 0.1 ! wetted fraction of fuel surface
* FFWLO 0.1 ! wetted fraction of MCO wall
* FFWLO 1.0 ! mass of sludge particles (kg) in the fuel basket
* MSISC 45.0 ! 22.5 kg per fuel basket x 2 basket = 45 kg
* view factor matrix between the insert,
* outer surface of outer fuel element,
* and the MCO wall. Therefore, the dimension of the square matrix is
* ! number of fuel rods2. If there is no insert, number of fuel
* rods2.
* FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.316 0.316 0.000 0.167 0.158 0.000 0.009 0.009
0.176 0.176 0.000 0.167 0.158 0.000 0.167 0.167
0.009 0.009 0.000 0.167 0.158 0.000 0.167 0.167
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
* gap distance for micro-convection calculation
* XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.037 0.037 0.037 0.056 0.000 0.000 0.000
0.037 0.037 0.037 0.037 0.037 0.037 0.037 0.037
0.056 0.056 0.037 0.037 0.037 0.037 0.037 0.037
0.000 0.056 0.037 0.037 0.037 0.056 0.037 0.056
0.000 0.056 0.000 0.037 0.037 0.056 0.037 0.056
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
* END IHSCF for 1st fuel basket
* END FUEL_BSKT
* SCRAP_BSKT 0 ! Total number of scrap baskets
* IHSC 31 ! ring 1, theta
32 33 ! ring 2, theta
34 35 ! ring 3, theta
36 36 ! ring 4, theta
37 37 ! ring 5, theta
38 38 ! ring 6, theta
39 39 ! ring 7, theta
* ICSINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
* ICSFIN 40 ! define copper fin heat sink

```

```

ACTIVE MODELS      : Keyword; MODELS is a comment; 1 = on, 0 = off
IJUNC 0           : Junction flow model
ICFJW 0           : Counter-current flow model
IRSHK 1           : Heat sinks
IRNDN 0           : Condensation
IRADS 0           : Aerosol Sedimentation
ITLEAK 0          : Aerosol Leakage
IFOGS 0           : Fog formation
ISRC 0            : User-defined sources
IMCO 1            : MCO models
ISNS 0           : Sensitivity runs
END ACTIVE MODELS : ACTIVE MODELS is a comment

SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
ENTER: TIME, TEMP, FLOWRATES, POWER
SYNTAX EXAMPLE:
SOURCES 2         : 1 -- KEYWORD AND # SOURCE GROUPS
REGION 1 GASES 2 : 1-- REGION #, # GASES
STEAM HYDROGEN   : 1-- GAS NAMES MUST BE ON NEXT LINE
0 300 1.E-3      : 1.E-3 0.E0
10 300 1.E-3     : 1.E-3 0.E0
END REGION
REGION -1 GASES 1
NAZO
0 300.0 4.44E-1 0.E0
10 300.0 4.44E-1 0.E0
900 300.0 4.44E-1 0.E0
901 300.0 0.E0 0.E0
1.E5 300.0 0.E0 0.E0
END REGION
END SOURCE
1-- ENDS A REGION SOURCE
1-- ENDS ALL SOURCE INPUT

END CONTROL      : End of CONTROL keyword group

VOLUMES 1        : total number of control volumes
REGIONS 1
GASNAME 1.0
SPD AREA 0.0
ELEVATION 0.0
TEMP GAS 299.15
PRESSURE 1.E5
END REGIONS

* Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
GASES 1
HELIUM 0.8

```

[illegible]

Date: 12/31/98


```

* * fraction of geometric area exposed for oxidation
* * = area available for oxidation/total heat sink area
* *
* * FAOMFL 0.036 0.036 0.036 0.036 0.036 0.036 0.036
* * FOX 0.036 0.036 0.036 0.036 0.036 0.036 0.036
* * XFLMO 0.01 ! initial oxide (oxide+hydride) thickness (to be
* * applied to
* * : exposed area)
* * FWHYD 1.0 ! fraction of initial oxide which is hydride
* *
* * Initial amount (kg) of water per geometric surface area (m2) of fuel
* * =  $8.6/2(16.58 + 0.256 \text{ kg/m}^2 \times 35 \text{ (per side)})$ 
* * FWHIO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* * FWHLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* * FWHLO 0.0 ! on the outer surface of the insert
* * FWHLO 0.0 ! on the inner surface of the MCO wall
* * FWHLO 0.0 ! wetted fraction of fuel surface
* * FWHLO 1.0 ! wetted fraction of MCO wall
* * MSLEFL 45.0 ! mass of sludge particles (kg) in the fuel basket
* * ! 22.5 kg per fuel basket x 2 basket = 45 kg
* *
* * view factor matrix between the insert,
* * outer surface of outer fuel elements,
* * and the MCO wall. Therefore, the dimension of the square matrix is
* * = number of fuel rods+1. If there is no insert, number of fuel
* * rods+1.
* * FVIEW 0.492 0.316 0.176 0.069 0.000 0.000 0.000 0.000
* * 0.116 0.316 0.006 0.167 0.009 0.009 0.000 0.000
* * 0.018 0.316 0.334 0.167 0.316 0.316 0.167 0.022
* * 0.000 0.018 0.158 0.158 0.000 0.018 0.158 0.107
* * 0.000 0.009 0.000 0.158 0.018 0.000 0.158 0.208
* * 0.000 0.000 0.018 0.167 0.316 0.316 0.048 0.558
* * 0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
* *
* * gap distance for micro-convection calculation
* * XGNP 0.000 0.037 0.037 0.037 0.000 0.000 0.000 0.000
* * 0.037 0.000 0.037 0.037 0.056 0.056 0.000 0.000
* * 0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000
* * 0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090
* * 0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.090
* * 0.000 0.056 0.000 0.037 0.037 0.037 0.037 0.090
* * 0.000 0.000 0.000 0.037 0.037 0.037 0.037 0.043
* * 0.000 0.000 0.000 0.030 0.030 0.030 0.056 0.043 0.000
* *
* * END INSET for 1st fuel basket
* * END INSET_BSKT
* *
* * SCRAP_BSKT 0 ! Total number of scrap baskets
* *
* * IHSSC 31 33
* * 32 35
* * 33 36
* * 37 36
* * 38 39
* * ! ring 1, theta
* * ! ring 2, theta
* * ! ring 3, theta
* * ! ring 4, theta
* * ! ring 5, radial
* * ! ring 6 & 5, radial
* * ! ring 11 & 12, radial

```

Uranium Oxidation Validation # 1

A.10A

```

* * FUEL CORROSION MODEL TEST: OXDPN1.DAT
* *
* *

```


1 2 3 4 5
0.0001 0.0 0.0 0.0 0.0

* AEROSOLS
* STEAM
* END AEROSOLS ! AEROSOLS is a comment

* No more than five columns at a time, so continue with 6 & 7

* AEROSOLS
* STEAM
* END AEROSOLS ! AEROSOLS is a comment

* OPTIONAL TEMPERATURE AND PRESSURE CONTROL

* CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE

* IMPOSE TEMPERATURE LOOK-UP TABLE

* SYNTAX:

* OFFSET_TIMEPG
* EXTRAPOLATION_TIMEPG
* TIMEPG REG TIME1, TIME2...TIMELAST
* TIMEPG REG TIME1, TEMP2...TEMPLAST
* TIMEPG REG PRES1, PRES2...PRESLAST
* LINEAR INTERPOLATION BETWEEN VALUES

* SIMILAR SYNTAX FOR PRESSURE:

* OFFSET_TIMEPG
* EXTRAPOLATION_TIMEPG
* TIMEPG REG TIME1, TIME2...TIMELAST
* TIMEPG REG PRES1, PRES2...PRESLAST
* PREX REG TIME1, TIME2...TIMELAST
* PREX REG PRES1, PRES2...PRESLAST

* OFFSET_TIMEPG* TIME-OFFSET_TIMEPG LAST TO USE LAST VALUE IN THE TABLE,
* EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
* = PERIOD TO WRAP AROUND.

* OFFSET_TIMEPG
* EXTRAPOLATION_TIMEPG
* TIMEPG REG TIME1, TIME2...TIMELAST
* TIMEPG REG PRES1, PRES2...PRESLAST
* TIMEPG REG TIME1, TIME2...TIMELAST
* TIMEPG REG PRES1, PRES2...PRESLAST

* CONTROL MCO BOUNDARY P, 30.
* EXTRAPOLATION_TIMEPG
* TIMEPG REG TIME1, TIME2...TIMELAST
* TIMEPG REG PRES1, PRES2...PRESLAST
* PREX REG TIME1, TIME2...TIMELAST
* PREX REG PRES1, PRES2...PRESLAST

* END VOLUMES ! VOLUMES is a comment

* Major keyword-- 44 ! Total number of heat sinks

* HENT SINKS

* decay power based on 835 W Per MCO.

* No more than 5 columns at a time,

* Repeat the following structure,

* SINKS

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

* .

Date: 12/31/98

A - 24

* 901. 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

* 1.25 300.0 0.50 0.50

FAI/98-40, Rev. 1

[illegible]

A - 28

[illegible]


```

* characteristic size for each scrap heat sink in the order read in (m)
XDCSRP 0.00635 0.00635 0.00635 0.00635 0.00635
XDCSRP 0.0254 0.0254 0.0254 0.0254
XRCBCK 0.2860 1 radius of scrap basket (m)
XHCBCR 0.691 1 height of scrap basket (m)

* exposed surface area available for oxidation
* each scrap basket heat sink in the order read in
* Example:
* 6 m2 bounding oxidation area: 6/0.17491 = 34.30 m2
* 10 m2 fine oxidation area: 10/0.01756 = 569.46 m2/m3
* 5.4 m2 coarse oxidation area: 5.4/0.15734 = 34.32 m2/m3

AVXMSC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
FOXSC 10 0.0 0.0 multiplier for AVXMSC
ASXCOX 0.0 1 initial oxide thickness on the exposed surface (m)

FSCHYD 0.0 1 fraction of oxide which is hydrate
* 1.5 kg of water total for scrap basket; 1.5/0.17491 = 8.576 kg/m3
* MWNSCO 8.576 1 initial amount (kg) of water per unit bulk volume
MWNSCO 0.

FNSCIO 0.0 1 (m3) of scrap
1 on the outer surface of the insert
1 on the inner surface of the MCO wall
FNSCHM 0.0 1 (per unit area, m2)
FANSC 0.1 1 wetted fraction of surface area
FANSCM 1.0 1 wetted fraction of MCO wall
XSCINS 0.01 1 gap distance between the insert and scrap basket
1 1/4" gap for scrap basket and MCO wall
XSCMCO 0.00635 1 gap distance between scrap basket and MCO wall
MSLSC 55.0 1 mass of sludge particles (kg) in the scrap basket
END IHSCF for 1st scrap basket
END SCRAE_BSKT
END MCO

```

A.10B Uranium Oxidation Validation # 2

```

*****
FUEL CORROSION MODEL TEST: OXDTN1.DAT
*****
T-300 C. MOIST & OXYGENATED AIR IN MCO, NO HEAT DIVERSION TO GAS,
NO CONDENSATION/EVAPORATION
UNLESS OTHERWISE NOTED, MKS UNITS
- 1 TIER OF SCRAP BASKET
- 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
*****
CONTROL 1 Major keyword group

```

```

* TITLE 1 Keyword; next line is title, title can be any length
FUEL CORROSION AT 300 C IN OXYGENATED GAS
END TITLE 1 Anything after END is a comment

* TIMING 1 Keyword
TSTART 0. 1 START TIME, >0 FOR RESTART RUN
1 RESTART FILE IS READ FROM HANSF.RER
1 END TIME (Seconds)
1 MIN TIMESTEP (Seconds)
DTMIN 0.001
DTMAX 0.001
1 PRINT INTERVAL (Seconds)
PTMIN 10.
PTMAX 100.
1 MAX INTERVAL (Seconds)
1 MIN INTERVAL (Seconds)
1 MAX INTERVAL (Seconds)
1 MIN INTERVAL (Seconds)
1 FRACTIONAL CHANGE IN T AND P
1 FRACTIONAL CHANGE IN AEROSOL MASS
1 FRACTIONAL CHANGE FOR PLOTTING
END TIMING 1 TIMING is a comment.

```

1 Keyword for plotting section

* Plotting syntax:

```

* PRESSURE n rlist - Pressure, Pa
* GAS-T n rlist - Gas Temperature, K
* HS-T n rlist - Heat Sink Temperature - Inner Surface, K
* HS-TO n rlist - Heat Sink Temperature - Outer Surface, K
* HS-TA n rlist - Heat Sink Temperature - Average, K
* AEROSOL n rlist - Aerosol Mass (Total), kg
* GAS-W n rlist - Mass Flowrate, kg/s
* GAS-WX n rlist - Counter-current Mass Flowrate, kg/s
* GAS-X n rlist - Gas Molar Fraction, Humidity
* GAS-RH GASNAME n rlist - Gas Mass (Species), kg
* GAS-HMS GASNAME n rlist - Aerosol Mass (Species), kg
* MAS GASNAME n rlist - Total Mass (Species), kg
* MAS GASNAME n rlist - Deposited Mass (Species), kg
* LIQ-HMS GASNAME n rlist - Deposited Mass (Species), kg

* Pressure, Gas Temperature, and total aerosol mass require a region
* list

```

* Heat Sink Temperatures need a heat sink number list

* Flowrates need a junction number list

* Gas concentration, relative humidity, individual species gas mass, individual species aerosol mass, total (gas+aerosol) individual species mass, and individual species deposited liquid mass require a region and gas name

```

PRESSURE 1 1 2 3 4 5 1 Pressure in MCO
GAS-T 1 31 32 33 34 35 36 37 38 39 40 41 Scrap basket
HS-T 1 42 43 44 45 46 47 48 49 50 Cask, bottom, and lid
HS-TA 10 1 2 3 4 5 6 7 8 9 10 Mid. fuel
HS-TA 5 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 Bot. fuel
HS-TA 10 16 17 18 19 20 21 22 23 24 25 Bot. fuel

```

Units: SED_AREA m², ELEVATION m, TEMP GAS K, PRESSURE Pa
 * VOLUME m³, SED_AREA m², ELEVATION m, TEMP GAS K, PRESSURE Pa
 * MCO top MCO middle MCO bottom gap environment
 * REGIONS 1 0.183 0.183 0.183 0.25 1.29
 * VOLUME 0.183 0.172 0.172 0.0 0.0
 * SED_AREA 2.65 1.33 300.00 300.00 300.00
 * ELEVATION 300.00 300.00 300.00 1.000E5 1.000E5
 * TEMP 1.000E5 1.000E5 1.000E5 1.000E5 1.000E5
 * PRESSURE 1.000E5 1.000E5 1.000E5 1.000E5 1.000E5
 * END REGIONS 1 REGIONS is a comment
 * If there are more than five regions, continue here
 * REGIONS 7
 * VOLUME 0.183 1.29 0.0
 * SED_AREA 0.27 0.0 0.0
 * ELEVATION 323.15 299.85 0.0
 * TEMP 1.047E5 1.047E5 0.0
 * PRESSURE 1.047E5 1.047E5 0.0
 * END REGIONS 1 REGIONS is a comment
 * Gas composition of each region; specify mole fraction of each gas
 * No more than five columns at a time
 * GASES 1 2 3 4 5
 * HELIUM 0.00 0.00 0.00 0.00 0.00
 * STEAM 0.01 0.01 0.01 0.01 0.01
 * NITROGEN 0.20 0.20 0.20 0.20 0.20
 * NITROGEN 0.79 0.79 0.79 0.79 0.79
 * END GASES
 * If there are more than five regions, continue here.
 * GASES 7
 * HELIUM 0.0 0.0
 * STEAM 0.11 0.0156
 * OXYGEN 0.0 0.2067
 * NITROGEN 0.0 0.7775
 * NITROGEN 0.0 0.0
 * END GASES 1 GASES is a comment
 * Aerosol concentration of each region (kg/m³)
 * No more than five columns at a time
 * AEROSOLS 1 2 3 4 5
 * STEAM 0.0001 0.0 0.0 0.0 0.0
 * END AEROSOLS 1 AEROSOLS is a comment
 * No more than five columns at a time, so continue with 6 & 7
 * AEROSOLS 6 7
 * STEAM 0.0 0.0
 * END AEROSOLS 1 AEROSOLS is a comment
 * OPTIONAL TEMPERATURE AND PRESSURE CONTROL
 * CONTROL MCO GROUP GASES AND MCO INLET GAS TEMPERATURE
 * IMPOSE TEMPERATURE LOOK-UP TABLE
 * SINTX!

Date: 12/31/98

A - 31

HS-PA 5 26 27 28 29 30
 GAS-X NITROGEN 3 1 2 3 1 N2 concentration in MCO
 GAS-X STEAM 3 1 2 3 1 O2 concentration in MCO
 GAS-X STEAM 3 1 2 3 1 H2O concentration in MCO
 GAS-X HYDROGEN 3 1 2 3 1 He concentration in MCO
 GAS-X HELIUM 3 1 2 3 1 Uni-directional mass flowrate
 GAS-W 3 1 2 3 1 Counter-current mass flowrate
 GAS-WX 3 1 2 3 1 Mass of hydrogen in region 5
 GAS-MASS HYDROGEN 1 5 1 Mass of steam in region 5
 GAS-MASS STEAM 1 5 1
 END PLOT 1 PLOT is a comment
 * ACTIVE MODELS 1 Keyword; MODELS is a comment; 1 = on, 0 = off
 * JUNCTION 1 Junction flow model
 * ICFLOW 1 Counter-current flow model
 * ITHINK 1 Heat sink
 * ICNDS 0 Condensation
 * ICNDS 0 Aerosol Sedimentation
 * ICNDS 0 Aerosol Leakage
 * IFAEK 0 Fog formation
 * IPOFO 0 User-defined sources
 * ISRC 0 MCO models
 * IMCO 0 Sensitivity runs
 * IMRS 0 Active MODELS is a comment
 * END ACTIVE MODELS 1 ACTIVE MODELS is a comment
 * C
 * C SOURCE GROUP: GROUPS REPEATED FOR INPUT 1 OF REGIONS
 * C END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
 * C END OF TIME, TEMP, FLOWRATES, POWER
 * C SINTX EXAMPLE:
 * C 1 --- KEYWORD AND # SOURCE GROUPS
 * C 1 --- REGION #, # GASES
 * C 1 --- GAS NAMES MUST BE ON NEXT LINE
 * C SOURCES 2
 * C REGION 1 GASES 2
 * C STEAM HYDROGEN 1-E-3 1-E-3 0.0
 * C 10 300 1-E-3 1-E-3 0.0
 * C 10 300 1-E-3 1-E-3 0.0
 * C 1 --- ENDS A REGION SOURCE
 * C 1 --- FOR AEROSOL, SPECIFY -IVE REGION
 * C REGION -1 GASES 1
 * C NAZO 300.0 4.44E-1 0.0
 * C 10 300.0 4.44E-1 0.0
 * C 10 300.0 4.44E-1 0.0
 * C 900 300.0 4.44E-1 0.0
 * C 901 300.0 0.0 0.0
 * C 1.25 300.0 0.0 0.0
 * C 1 --- ENDS A REGION SOURCE
 * C 1 --- ENDS ALL SOURCE INPUT
 * C END REGION
 * C END SOURCE
 * C
 * C END CONTROL 1 End of CONTROL keyword group
 * C
 * C
 * C VOLUMES 5 1 total number of control volumes
 * C 1 total MCO gas volume is 0.55 m³, 0.55/3=0.183 per each node
 * C No more than 5 columns (regions) at a time

A - 32

FAI/98-40, Rev. 1

A - 33


```

XHYD2      1.0      ! H2O/U ratio (stoich. number) to switch
              from first to second correlation
XHYD3      0.5      ! H2O/U ratio (stoich. number) to switch
              from second to third correlation
AHEQ01     18.012   ! 'A' IN LN P = A + B/T FOR X > XHYD2
SHEQ01     -6775.E0 ! 'B' IN LN P = A + B/T FOR X > XHYD2
AHEQ02     19.076   ! 'A' IN LN P = A + B/T FOR X < XHYD2
SHEQ02     -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD2
AHEQ03     19.076   ! 'A' IN LN P = A + B/T FOR X < XHYD3
SHEQ03     -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHYD3
AHEQ04     19.076   ! 'A' IN LN K = A + B/T FOR X > XHYD2
SHEQ04     -8312.E0 ! 'B' IN LN K = A + B/T FOR X > XHYD2
ADEH01     5.2295E0 ! 'A' IN LN K = A + B/T FOR X < XHYD2
BOEHY1     -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD2
ADEH02     5.2295E0 ! 'A' IN LN K = A + B/T FOR X < XHYD2
BOEHY2     -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD2
ADEH03     5.2295E0 ! 'A' IN LN K = A + B/T FOR X < XHYD3
BOEHY3     -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHYD3
DEHY1      3.7056    ! Decomposition enthalpy J/kg H2O: 1st step
DHNY1      3.7056    ! Decomposition enthalpy J/kg H2O: 2nd step
DHNY2      3.7056    ! Decomposition enthalpy J/kg H2O: 3rd step
PEOHY1     1.0       ! Hydrate production rate law multiplier
PCOHY1     1.0       ! Hydrate consumption rate law multiplier
FCOHY1     1.0       ! Nitriding rate law multiplier
FNTRI1     1.0       !
*****
PUMP, FEED, AND CONDENSE MODELS
Syntax:
**** PUMP IRUPM IROPUM ICONPM INFEE WVPUMP WFEED TGFEE TCOPNP
*****
Definitions:
IRUPM = Pump inlet region
IROPUM = Pump outlet region
ICONPM = Node to which the condensed steam is dumped for book-keeping
INFEE = Feed volumetric flowrate (m3/s)
WVPUMP = Condenser cooling coil temperature (K)
WFEED = Feed temperature (°C)
TGFEE = Feed temperature (°C)
TCOPNP = Condenser cooling coil temperature (K)
*****
temperature
WVPUMP = Pump volumetric flowrate (m3/s)
WFEED = Feed volumetric flowrate (m3/s)
TGFEE = Feed temperature (°C)
TCOPNP = Condenser cooling coil temperature (K)
*****
35 FT3/MIN * 1 MIN/60 SEC * 0.02832 M3/l FM3 = 0.01652 M3/SEC
PUMP1      1        ! PUMP IRUPM IROPUM ICONPM INFEE WVPUMP WFEED TGFEE TCOPNP
PUMP1      5        !          0          0          1.652E-2 0.0 0.0 0.0
*****
Radiolyse parameters
*****
FRAD       1.0       ! multiplier for radiolysis
FALPHA     0.197     ! alpha fractional heat load
FBETA      0.486     ! beta fractional heat load
FFEPA      0.317     ! gamma fractional heat load
FGAMA      2.4E-6    ! positron deposition rate in MCO free water per gram
QPHOTO     2.4E-6    ! per MTU of fuel loading
*****
! GENERAL is a comment
*****
END GENERAL
*****
** SOLAR_BAD
** pointers to heat sinks representing the cask wall and the top
** solar radiation impinges on these
*****
IFCASK     42

```

A - 35-

END JUNCTIONS	JUNCTIONS IS A COMMENT.
MCO	MCO Major Keyword
GENERAL	Keyword for general inputs
IOXPTN 1	-1, oxidation of fuel/acrap
IHYD 0	-1, disable oxidation of fuel/acrap
IHYDR 0	-1, do hydriding/dehydriding calculation
IHWRT 0	-1, disable hydriding/dehydriding calculation
IHWRT 0	-1, divert heat transfer to gas to gas
IWAV 0	-1, do not divert heat transfer to water
IWLAW 0	-1, do evaporation/condensation
IWLAW 1	-1, do not do evaporation/condensation
IDENT 0	oxidation rate law, 1 - Pecorre
IENR 0	-1, de-entrainment of aerosol due to scrap basket
IHYDRA 0	-1, disablentrainment calculation
INTRI 0	-1, do sludge entrainment calculation
IRADTIO 0	-1, do decomposition of fuel oxide hydrate
XHYD 5.E-5	-1, disable hydrate decomposition calculation
IHSCK 42	-1, do nitrating calculation
IRGAP 4	-1, disable radiolytic calculation
	-1, average diameter coat sink
	-1, define the crack node (between MCO wall and the crack)
	-1, define the gap node (between the MCO wall and the radiative/conductive h.t. between the MCO wall and the crack is computed and some of the heat is
diverted	to gas for stability
XGPCSK 0.0155	gap distance between the MCO wall and the crack
FHTLID 0.0	-1, turn off the radiative heat transfer between the fuel/acrap and the lid/floor
RHOSL 5000.	-1, fully account for the relative heat transfer
SAS 1000.	sludge particle density (kg/m^3)
MOSE 1.E-6	sludge specific area (m^2/mg)
	sludge particle diameter. (m)
* Hydrate Model:	two-step decomposition,
* input curves for ln P and ln X	
* first step for x > XHYD1, second step for x < XHYD2 .	
* 10 % weight fraction of sludge being water is equivalent to 90 %	
* of sludge being hydrated with 2 moles of	
* water per mole of uranium oxide	
* FHYSL 0.9	fraction of sludge that is hydrated
XHYSL 2.0	stoichiometry number of hydrate (moles of water per mole of uranium oxide (UO ₃ H ₂ O))

Date: 12/31/98

A - 36

FAI/98-40, Rev. 1

INTOP 44

* look-up table for solar radiation throughout a day (sec. vs. W/m^2)

* OFFSET_TMDAY 21600, ! offset by six hours

* EXTRAPOLATION_TMDAY PERIOD, ! repeat the diurnal cycle

* TMDAY 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0

25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0

50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0

75600.0 79200.0 82800.0 86400.0

* RAD SUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0

* END SOLAR_RAD

* FUEL_BSKT 2 ! Total number of fuel baskets

* 1st Fuel Basket

* IHSELF 1 2 3 4 5 6 7 8 9 10 11 12 13 14

! define the heat sinks comprising the first fuel basket (must be

! in pairs, for inner and outer elements)

* IFILINS 0 ! define the adjacent center insert heat sink,

0 for no insert

* IFIMCO 15 ! define the adjacent MCO wall heat sink

! define the lid or floor heat sink to which the fuel

IFILID 0

* AFLEL 0.131 ! flow area in the basket

* fraction of geometric area exposed for oxidation

* = area available for oxidation/total heat sink area

* 6.8 m² / (2+33.6 m²) = 0.10119

FAOXFL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

FOX 0.0 0.0 ! multiplier for FAOXFL

XFOXLO 0.0 ! initial oxide (oxide-hydride) thickness

! (to be applied to exposed area)

* FXHYD0 0.0 ! fraction of initial oxide which is hydride

* initial amount (kg) of water per geometric surface area (m²) of fuel

* 24 kg / (2+33.6 m²) = 0.3571 (side)

* 8.6/2/16.8 = 0.2539/m² (top)

* FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

* FWELIO 0.0 ! on the outer surface of the insert

0.0 ! on the inner surface of the MCO wall

* FWELMO 0.0 ! on the inner surface of the MCO wall

0.0 ! wetted fraction of fuel surface

* FANFLM 0.1 ! wetted fraction of MCO wall

1.0 ! mass of sludge particles (kg) in the fuel basket

MSLEFL 45.0 ! 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,

* outer surface of outer fuel elements,

* and the MCO wall. Therefore, the dimension of the square matrix is

* 1=number of fuel rods+1. If there is no insert, number of fuel

* rods+1.

* FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000 0.000

0.316 0.027 0.316 0.158 0.018 0.009 0.000 0.000 0.000

0.176 0.316 0.000 0.167 0.158 0.009 0.000 0.000 0.000

0.018 0.316 0.334 0.167 0.316 0.316 0.167 0.022

0.000 0.316 0.158 0.158 0.000 0.000 0.158 0.107

0.000 0.009 0.000 0.159 0.018 0.000 0.158 0.558

0.000 0.000 0.018 0.167 0.176 0.316 0.460

0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106

* gap distance for micro-convection calculation

* XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000

0.037 0.000 0.037 0.037 0.056 0.000 0.000 0.000

0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000

0.056 0.037 0.037 0.000 0.037 0.056 0.037 0.090

0.000 0.056 0.000 0.037 0.056 0.000 0.037 0.056

0.000 0.000 0.037 0.037 0.037 0.037 0.000 0.043

0.000 0.000 0.000 0.037 0.037 0.037 0.000 0.043

END IHSELF for 1st fuel basket

* 2nd Fuel Basket

* heat sink pairs for second fuel basket

* IHSELF 16 17 18 19 20 21 22 23 24 25 26 27 28 29

! define the adjacent center insert heat sink,

IFILINS 0 ! 0 for no insert

* IFIMCO 30 ! define the adjacent MCO wall heat sink

! define the lid or floor heat sink to which the fuel

IFILID 43 ! radiate to

* AFLEL 0.131 ! flow area in the basket,

* fraction of geometric area exposed for oxidation

* 6.8 m² / (2+33.6 m²) = 0.10119

FAOXFL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

FOX 10.0 ! multiplier for FAOXFL

XFOXLO 0.0 ! initial oxide (oxide-hydride) thickness

! (to be applied to exposed area)

* FXHYD0 0.0 ! fraction of initial oxide which is hydride

* initial amount (kg) of water per geometric surface area (m²) of fuel

* 24 kg / (2+33.6 m²) = 0.3571 (side)

* 8.6/2/16.8 = 0.2539/m² (top)

* FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

* FWELIO 0.0 ! on the outer surface of the insert

0.0 ! on the inner surface of the MCO wall

* FWELMO 0.4545 ! on the inner surface of the MCO wall

0.4545 ! wetted fraction of fuel surface

* FANFLM 1.0 ! wetted fraction of MCO wall

1.0 ! mass of sludge particles (kg) in the fuel basket

MSLEFL 45.0 ! 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,

* outer surface of outer fuel elements,

* and the MCO wall. Therefore, the dimension of the square matrix is

* 1=number of fuel rods+1. If there is no insert, number of fuel

* rods+1.

```

* 1=number of fuel rods+1. If there is no insert, number of fuel
* rods+1.
*
FVWFM 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000 0.000
0.316 0.027 0.316 0.158 0.018 0.000 0.000 0.000 0.000
0.176 0.036 0.000 0.167 0.016 0.000 0.009 0.000 0.000
0.316 0.316 0.158 0.316 0.316 0.158 0.022 0.107
0.018 0.316 0.158 0.158 0.000 0.018 0.158 0.107
0.000 0.018 0.000 0.158 0.018 0.000 0.158 0.208
0.000 0.000 0.000 0.158 0.018 0.000 0.158 0.558
0.000 0.000 0.018 0.167 0.316 0.316 0.448 0.558
0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106

*
* gap distance for micro-convection calculation
*
XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000 0.000
0.037 0.000 0.037 0.037 0.056 0.056 0.056 0.037 0.000
0.037 0.037 0.037 0.037 0.037 0.037 0.037 0.037 0.090
0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.037 0.056
0.000 0.056 0.037 0.037 0.056 0.000 0.037 0.037 0.056
0.000 0.000 0.037 0.037 0.037 0.037 0.037 0.000 0.043
0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.043 0.000

END IHSEL for 2nd fuel basket
END FUEL_BSKT
*
SCRAP_BSKT 1 ! Total number of scrap baskets
*
IHSSC 31 ! ring 1; theta
32 33 ! ring 2; theta
34 35 ! ring 3 & 4, radial
37 36 ! ring 6 & 5, radial
38 39 ! ring 11 & 12, radial

*
ISCINS 0 ! define the adjacent center insert heat sink,
! for no insert
ISCFTN 40 ! define copper fin heat sink
ISCMCO 41 ! define the adjacent MCO wall heat sink
ISCLID 44 ! define the lid or floor heat sink to which the
scrap
! radiate to
*
porosity of the scrap for each heat sink in the order read in
*
(31, 32, 33, 34, 35) 0.45 0.45 0.45 0.6 0.6 0.6 0.6
*
FPORES 0.45 ! porosity of the scrap for each heat sink in the order read in (m)
*
characteristic size for each scrap heat sink in the order read in (m)
*
XSCGRP 0.00635 0.00635 0.00635 0.00635 0.00635 0.00635
0.0254 0.0254 0.0254 0.0254 0.0254
*
XSCBCK 0.2860 ! radius of scrap basket (m)
XSCBCK 0.691 ! height of scrap basket (m)
*
exposed surface area available for oxidation
*
per unit volume of scrap (1/m3) for
*
each scrap basket heat sink in the order read in
*
EASAP 6.0 ! exposed surface area available for oxidation
6 m2 bounding oxidation area: 6/0.17491 = 34.30 m2
*
10 m2 fine oxidation area: 10/0.01756 = 569.48 m2/m3
*
5.4 m2 coarse oxidation area: 5.4/0.15734 = 34.32 m2/m3
*
AVOMSC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
FOVSC 10.0 ! multiplier for AVOMSC

```

A.10C Uranium Oxidation Validation # 3

```

*****
* FUEL CORROSION MODEL TEST: OMDTNS.DMT
*
T=75 C, MOIST & OXYGEN FREE AIR IN MCO, NO HEAT DIVERSION TO GAS,
NO CONDENSATION/EVAPORATION
UNLESS OTHERWISE NOTED, MKS UNITS
- 1 TIER OF SCRAP BASKET
- 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
*****
*****
CONTROL ! Major keyword group
*****
*
* TITLE ! Keyword; next line is title, title can be any length
FUEL CORROSION AT 75 C IN OXYGEN FREE GAS
END TITLE ! Anything after END is a comment
*
*
TIMING ! Keyword
TSTART 0.
TEND 1000.
TMIN 0.01
TMAX 250.
PRINT INTERVAL (Seconds)
! START TIME, >0 FOR RESTART RUN
! RESTART FILE IS READ FROM HANSF.RER
! END TIME (Seconds)
! END TIME STEP (Seconds)
! MAX TIME STEP (Seconds)
! PRINT INTERVAL (Seconds)

```


Date: 12/31/98

```

ACTIVE MODELS ! Keyword; MODELS is a comment; 1 - on, 0 - off
IUNC 1 ! Junction flow model
ICF1W 1 ! Counter-current flow model
ICF1M 1 ! Counter-current flow model
INSINK 1 ! Sink
CONDENSATION 1 ! Condensation
AEROSOL 0 ! Aerosol Sedimentation
TALEAK 0 ! Aerosol Leakage
IFOG 0 ! Fog formation
ISRC 0 ! User-defined sources
IWC 1 ! MCO models
ISENS 0 ! Sensitivity runs
END ACTIVE MODELS ! ACTIVE MODELS is a comment

*
*
*
C
C SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
C END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
C ENTER: TIME, TEMP, FLOWRATES, POWER
C SYNTAX EXAMPLE:
C SOURCES 2 1 --- KEYWORD AND # GASES
C REGION 1 GASES 2 1 --- REGION #, # GASES
C STEAM HYDROGEN 1 --- GAS NAMES MUST BE ON NEXT LINE
C 0 300 1.0 1.0 0.0
C 0 300 1.0 1.0 0.0
C 0 300 1.0 1.0 0.0
C END REGION 1 --- ENDS A REGION SOURCE
C END REGION 1 --- ENDS ALL SOURCE INPUT
C END SOURCE
C END CONTROL ! End of CONTROL keyword group

*
*
*
VOLUMES 5 ! total number of control volumes
* total MCO gas volume is 0.55 m^3, 0.55/3=0.183 per each node
* Units:
* VOLUME m^3, SED_AREA m^2, ELEVATION m, TEMP_GAS K, PRESSURE Pa
* REGION 1 MCO top MCO middle MCO bottom gap environment
* VOLUME 0.183 0.183 0.183 0.25 1.0
* SED AREA 0.172 0.172 0.172 0.0 0.0
* ELEVATION 1.33 1.33 1.33 0.0 0.0
* TEMP_GAS 75.00 75.00 75.00 75.00 75.00
* PRESSURE 1.000E5 1.000E5 1.000E5 1.000E5 1.000E5
END REGIONS ! REGIONS is a comment
* If there are more than five regions, continue here.

```

A 38

FAI/98-40, Rev. 1

Date: 12/31/98

A - 39

FAU98-40, Rev. 1

```

* * * * *
* * REGIONS 6 7
* * VOLUME 0.183 1.1E9
* * SED AREA 0.27 0.0
* * ELEVATION 0.0 0.0
* * TEMP GAS 323.15 299.85
* * PRESSURE 1.047E5 1.047E5
* * END REGIONS 1 REGIONS is a comment
* * Gas composition of each region; specify mole fraction of each gas
* * No more than five columns at a time
* * * * *
* * GASES 1 2 3 4 5
* * HELIUM 0.00 0.00 0.00 0.0 0.0
* * STEAM 0.51 0.51 0.51 0.0 0.01
* * OXYGEN 0.00 0.00 0.00 0.20 0.78
* * NITROGEN 0.49 0.49 0.49 0.79 0.78
* * END GASES
* * If there are more than five regions, continue here.
* * * * *
* * GASES 6 7
* * HELIUM 0.89 0.0
* * STEAM 0.11 0.0158
* * OXYGEN 0.0 0.2067
* * NITROGEN 0.0 0.7775
* * WATER 0.0 0.0
* * END GASES 1 GASES is a comment
* * Aerosol concentration of each region (kg/m^3)
* * No more than five columns at a time
* * * * *
* * AEROSOLS 1 2 3 4 5
* * STEAM 0.0001 0.0 0.0 0.0 0.0
* * END AEROSOLS 1 AEROSOLS is a comment
* * No more than five columns at a time, so continue with 6 & 7
* * * * *
* * AEROSOLS 6 7
* * STEAM 0.0 0.0
* * END AEROSOLS 1 AEROSOLS is a comment
* * OPTIONAL TEMPERATURE AND PRESSURE CONTROL
* * CONTROL MCO HEATUP GASES AND INLET GAS TEMPERATURE
* * IMPUSE TEMPERATURE LOOK-UP TABLE
* * * * *
* * OFFSET TIMETG
* * EXTRAPOLATION TIMETG
* * TIMEX IREG TIME1, TIME2...TIMELAST
* * TGPIX IREG TEMP1, TEMP2...TEMPLAST
* * LINEAR INTERPOLATION BETWEEN VALUES
* * * * *
* * SIMILAR SYNTAX FOR PRESSURE:
* * OFFSET TIMETG
* * EXTRAPOLATION TIMETG
* * TIMEX IREG TIME1, TIME2...
* * TGPIX IREG PRES1, PRES2...PRESSURES ARE IN PA1!!
* * * * *
* * PREFIX IREG TIME1, ENTER LOOKUP TABLE WITH
* * * * *

```

```

* * * * *
* * EXTRAPOLATION TIMETG= LAST TO USE LAST VALUE IN THE TABLE,
* * = PERIOD TO EXTRAPOLATE FROM LAST TWO POINTS,
* * = PERIOD TO WRAP AROUND.
* * * * *
* * OFFSET TIMETG 50.
* * EXTRAPOLATION TIMETG LAST
* * TIMEX 1 0.0 100. 200.
* * TGPIX 1 293.15 373.15 473.15
* * * * *
* * CONTROL MCO BOUNDARY P, 30.
* * * * *
* * EXTRAP
* * EXTRAPOLATION TIMETG 200.
* * TIMEP 1 0.0 100. 200.
* * PREFIX 1 1.1E5 1.2E5 1.4E5
* * * * *
* * END VOLUMES 1 VOLUMES is a comment
* * * * *
* * Major keyword----- 44 1 Total number of heat sinks
* * HEAT SINKS
* * * * *
* * decay power based on 835 W per MCO.
* * No more than 5 columns at a time,
* * Repeat the following structure,
* * * * *
* * SINKS
* * * * *
* * * * *
* * END
* * * * *
* * Syntax:
* * IGEOM 1 for plane, 0 or 2 for cylinder
* * RHO Density (kg/m^3)
* * KHS Thermal Conductivity (W/m/K)
* * CPHS Specific Heat (J/kg/K)
* * CV Volumetric Heat Generation (W/m^3)
* * XRI Inner Radius (m); for plane wall, thickness = XRO-XRI
* * XRO Outer Radius (m); for heat sink area (m^2)
* * XRI Initial inside surface temperature (C)
* * TIMINIT Initial outside surface temperature (C)
* * TIMSLAB Number of slabs; 3 is minimum
* * IREGI Region index for inner surface or 0 (insulated)
* * or -1 for constant temperature
* * ITHS Region surface temperature when IREGI = -1 (C)
* * IREGO Region index for outer surface or 0 (insulated)
* * or -1 for constant temperature
* * ITHO Region surface temperature when IREGO = -1 (C)
* * TCHS Characteristic length for natural convection (m)
* * XHS Characteristic length for natural convection (m)
* * EHSI Emissivity of inner surface
* * EHSO Emissivity of outer surface
* * * * *
* * decay power based on 835 W per MCO. 835/(0.3192+0.01756(1-0.45))+
* * 0.15734(1-0.6))=835/0.3918=2131 W/m^3
* * * * *
* * Fuel Basket #1 heat sinks 1 through 15: MCO MIDDLE
* * * * *

```


A 41

TMTWXS 15 2 0.0 1.56
TMSFX 15 2 75.0 75.0
TMTWSX 30 2 0.0 1.56
TMTWSX 30 2 75.0 75.0
TMTWSX 41 2 0.0 1.56
TMTWSX 41 2 75.0 75.0
TMTWSX 42 1 0.0 1.56
TMTWSX 42 1 75.0 75.0
TMTWSX 42 2 0.0 1.56
TMTWSX 42 2 75.0 75.0

END HEAT_SINKS ! HEAT_SINKS is a comment
JUNCTIONS 3 1 3 Junctions
* 1) MCO bottom to MCO middle, 3-->2
* 2) MCO middle to MCO top, 2->1
* 3) MCO top to Outlet volume, 1->5 (deactivated)

Syntax:
JTYPE: Junction Types: 1 = Normal, 2 = HEPA, 3 = Cover
IR1: Inlet Region
IR2: Outlet Region
DNSTRM: Downstream Region
AUN: Area (m²)
ABYP: Bypass area for HEPA Junction (m²)
AFILTR: HEPA Filter Failure Pressure (Pa)
ACOV: Cover Area (m²)
CWRGHT: Cover Weight (kg)
ELEVATION: Elevation at floor of IR1 opening (m)
LSS: Loss coefficient multiplies 0.5rho*v²
ORIENTATION: Orientation: 1 - horizontal, 0 - vertical
CHARACT: Characteristic width, m
CHARACT: Characteristic height, m
CHARACT: Characteristic length, m
DECONT: Decontamination factor
N90: No. of 90 bonds

	1	2	3
PATHS	1	2	3
IUTYV	1	1	1
IR1	3	2	5
IR2	2	1	5
IRHORZ	1	0.61	2.54E-2
XWIN	1.61	0.61	2.54E-2
XWIN	0.61	0.001	10.
XWIN	0.001	0.29	0.0
AUN'	1.29	1.2	10.
ZLN	0.0	0.0	12.65
ZLN	0.0	0.0	4.0
CJN	1.0	1.0	4.0
DFIN	1.0	1.0	3.0
N90	0	0	3

END PATHS ! PATHS is a comment.
END JUNCTIONS ! JUNCTIONS is a comment.
MCO Major Keyword

BOEHY1 -2546.E0 ! 'B' IN LN K = A + B/T FOR X > XHVD2
 ADHY21 -5.425E0 ! 'B' IN LN K = A + B/T FOR X < XHVD2
 ADHY31 -5.295E0 ! 'B' IN LN K = A + B/T FOR X < XHVD3
 ADHY31 -5.295E0 ! 'B' IN LN K = A + B/T FOR X < XHVD3
 BOEHY3 -2546.E0 ! 'B' IN LN K = A + B/T FOR X < XHVD3
 DHYV1 2.668E ! Decomposition enthalpy J/kg H2O: 1st step
 DHYV2 3.708E ! Decomposition enthalpy J/kg H2O: 2nd step
 DHYV2 3.708E ! Decomposition enthalpy J/kg H2O: 3rd step
 FPROY 1.0 ! Hydride production rate law multiplier
 FCONY 1.0 ! Hydride consumption rate law multiplier
 FNTY1 1.0 ! Initiating rate law multiplier

* PUMP, FEED, AND CONDENSER MODELS
 * SYNTAX:
 * PUMP IRUPM IROFPM ICONPM ITFEED WUPUMP WYFEED TGFEEED TCONPM
 * Definitions:
 * IRUPM = inlet region
 * IROFPM = pump outlet region
 * ICONPM = inlet/outlet region
 * TCONPM = Node to which the condensed steam is dumped for book-keeping
 * ITFEED = If non-zero, overrides TGFEEED with the designated region
 * temperature. Used to specified time-varying feed temperature
 * WUPUMP = Pump volumetric flowrate (m³/s)
 * WYFEED = Feed volumetric flowrate (m³/s)
 * TGFEEED = Feed temperature (K)
 * TCONPM = Condenser cooling coil temperature (K)
 * 35 FT³/MIN * 1 MIN/60 SEC * 0.02832 M³/1 FT³ = 0.01652 M³/SEC
 * PUMP IRUPM IROFPM ICONPM ITFEED WUPUMP WYFEED TGFEEED TCONPM
 * PUMP 1 5 0 0 1.652E-2 0.0 0.0 0.0

* Radiolysis parameters
 * FEND 1.0 ! multiplier for radiolysis
 * FALPHA 0.197 ! alpha fractional heat load
 * FBETA 0.486 ! beta fractional heat load
 * FGAMMA 0.317 ! gamma fractional heat load
 * QPHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
 * ! per MTU of fuel loading
 * ! GENERAL is a comment

* END GENERAL

* SOLAR RAD
 * pointers to heat sinks representing the cask wall and the top
 * solar radiation impinges on these
 * IHCASK 42
 * IHTOP 44

* Look-up table for solar radiation throughout a day (sec .vs. W/m²)
 * OFFSET TMDAY 21600. ! offset by six hours
 * EXTRAPOLATION TMDAY 21600. ! extrapolate diurnal cycle
 * TMDAY 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
 * 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
 * 75600.0 79200.0 82800.0 86400.0
 * 0.0 0.0 0.0 0.0 0.0 0.0 0.0

* RAD SUN

* FUEL_BSKT 2 ! Total number of fuel baskets
 * 1st Fuel Basket
 * IHSLF 1 2 3 4 5 6 7 8 9 10 11 12 13 14
 * ! define the heat sinks comprising the first fuel basket (must be
 * ! in pairs, for inner and outer elements)
 * ! IFLNS 0 ! define the adjacent center insert heat sink,
 * ! IFLMCO 15 ! define the adjacent MCO wall heat sink
 * ! IFLID 0 ! define the lid or floor heat sink to which the fuel
 * ! radiate to
 * ! APLFL 0.131 ! flow area in the basket
 * ! fraction of geometric area exposed for oxidation
 * ! - area available for oxidation/local heat sink area
 * 6.8 m² / (2*33.6 m²) = 0.10119
 * FNOXFL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
 * FOX 10 0.0 ! multiplier for FNOXFL
 * XFLOX0 0.0 ! initial oxide (oxide-hydride) thickness
 * ! (to be applied to exposed area)
 * FXHYD0 0.0 ! fraction of initial oxide which is hydride
 * ! initial amount (kg) of water per geometric surface area (m²) of fuel
 * 24 kg / (2*33.6 m²) = 0.3571
 * FWELO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
 * 8.6/2/16.8 = 0.256 kg/m² (per side)
 * FWELO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
 * FWELO 0.0 ! on the outer surface of the insert
 * FWELO 0.0 ! on the inner surface of the MCO wall
 * FWELO 0.1 ! wetted fraction of MCO wall
 * FWELO 1.0 ! wetted fraction of MCO wall
 * FWELO 45.0 ! weight of sludge particles (kg) in the fuel basket
 * ! 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,
 * outer surface of outer fuel elements,
 * and the MCO wall. Therefore, the dimension of the square matrix is
 * 1=number of fuel rods+1. If there is no insert, number of fuel
 * rods=1.
 * FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
 * 0.316 0.176 0.158 0.018 0.009 0.000 0.000 0.000
 * 0.176 0.316 0.000 0.167 0.158 0.009 0.000 0.000
 * 0.018 0.334 0.167 0.316 0.316 0.167 0.022 0.022
 * 0.000 0.018 0.158 0.000 0.158 0.000 0.158 0.107
 * 0.000 0.009 0.000 0.158 0.000 0.158 0.000 0.158
 * 0.000 0.000 0.000 0.158 0.167 0.316 0.316 0.048
 * 0.000 0.000 0.000 0.000 0.176 0.343 0.460 0.106

* gap distance for micro-convection calculation

A - 44

FAI/98-40, Rev. 1

A 10D Uranium Oxidation Validation # 4

major keyword group

```
* PLOT ! Keyword for plotting section
* Plotting syntax!
*
* PRESSURE n rlist - pressure, Pa
*                  c.c. memoraturo. K
```

FAI/98-40, Rev. 1

A - 45

FAI/98-40, Rev. 1

* If there are more than five regions, continue here.
 * GASES
 * HELIUM 1 2 3 4 5
 * STEAM 0.00 0.00 0.51 0.00 0.01
 * NITROGEN 0.00 0.00 0.00 0.20 0.20
 * NITROGEN 0.49 0.49 0.49 0.79 0.78
 * END GASES
 *
 * * If there are more than five regions, continue here.
 * * GASES
 * * HELIUM 6 7
 * * STEAM 0.89 0.00
 * * NITROGEN 0.11 0.0158
 * * NITROGEN 0.00 0.00
 * * WATER 0.00 0.7775
 * * WATER 0.00 0.00
 * * END GASES ! GASES is a comment
 * * Aerosol concentration of each region (kg/m³)
 * * No more than five columns at a time
 * * AEROSOLS 1 2 3 4 5
 * * STEAM 0.0001 0.0 0.0 0.0 0.0
 * * AEROSOLS ! AEROSOLS is a comment
 * * No more than five columns at a time, so continue with 6 & 7
 * * AEROSOLS 6 7
 * * STEAM 0.0 0.0
 * * AEROSOLS ! AEROSOLS is a comment
 * * OPTIONAL TEMPERATURE AND PRESSURE CONTROL
 * * TEMPERATURE AND PRESSURE INLET GAS TEMPERATURE
 * * TEMPERATURE LOOK-UP TABLE
 * * SYNTAX:
 * * EXTRAPOLATION TIMEG
 * * TIMEG IREG TIME1, TIME2...TIMELAST
 * * TGFX IREG TEMP1, TEMP2...TEMPLAST
 * * LINEAR INTERPOLATION BETWEEN VALUES
 * * SIMILAR SYNTAX FOR PRESSURE:
 * * EXTRAPOLATION TIMEG
 * * TIMEG IREG TIME1, TIME2...
 * * TGFX IREG PRES1, PRES2...PRESSURES ARE IN PA!!!
 * * OFFSET TIMEG- OFFSET TIME; ENTER LOOKUP TABLE WITH
 * * EXTRAPOLATION TIMEG- LAST TO USE LAST VALUE IN THE TABLE.
 * * - PERIOD TO INTERPOLATE FROM LAST TWO POINTS,
 * * - PERIOD TO WRAP AROUND.
 * * OFFSET TIMEG 50.
 * * EXTRAPOLATION TIMEG LAST
 * * TIMEG 1 0.0 100. 200.
 * * TGFX 1 293.15 373.15 473.15
 * * CONTROL MCO BOUNDARY P, 30.
 * * OFFSET TIMEG EXTRAP
 * * EXTRAPOLATION TIMEG EXTRAP

C-----
 C SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
 C END OF GROUP DESIGNATED BY 'REGION' OR 'END' ALIWORDS
 C ENTER: TIME, TEMP, FLOWRATES, POWER
 C SYNTAX EXAMPLE:
 C SOURCE 1 GASES 2 ! --- KEYWORD AND # SOURCE GROUPS
 C REGION 1 ! --- REGION #, # GASES
 C STEAM HYDROGEN ! --- GAS NAMES MUST BE ON NEXT LINE
 C 0 300 1.E-3 1.E-3 0.E0
 C 10 300 1.E-3 1.E-3 0.E0
 C END REGION
 C ! --- ENDS A REGION SOURCE
 C ! --- FOR AEROSOL, SPECIFY -IVE REGION
 C REGION -1 GASES 1
 C NAZO 0 300.0 4.44E-1 0.E0
 C 0 300.0 4.44E-1 0.E0
 C 4 300.0 4.44E-1 0.E0
 C 900 300.0 4.44E-1 0.E0
 C 901 300.0 0.E0 0.E0
 C 1.E5 300.0 0.E0 0.E0
 C END REGION
 C ! --- ENDS A REGION SOURCE
 C ! --- ENDS ALL SOURCE INPUT
 C END SOURCE
 C END CONTROL ! End of CONTROL keyword group
 C-----
 C-----
 C VOLUMES 5 ! total number of control volumes
 C * total MCO gas volume is 0.55 m³, 0.55/3=0.183 per each node
 C * No more than 5 columns (regions) at a time
 C Units:
 C * VOLUME m³, SED_AREA m², ELEVATION m, TEMP_GAS K, PRESSURE Pa
 C REGIONS 1 2 3 4 5
 C VOLUME 0.183 0.183 0.183 0.25 1.E9
 C SED AREA 0.172 0.172 0.172 0.0 0.0
 C ELEVATION 2.65 1.33 0.0 0.0 0.0
 C TEMP GAS 300.00 300.00 300.00 300.00 300.00
 C PRESSURE 1.000E5 1.000E5 1.000E5 1.000E5 1.000E5
 C END REGIONS ! REGIONS is a comment
 C * If there are more than five regions, continue here
 C REGIONS 6 7
 C VOLUME 0.183 1.E9
 C SED AREA 0.27 0.0
 C ELEVATION 0.0 0.0
 C TEMP GAS 323.15 299.85
 C PRESSURE 1.047E5 1.047E5
 C END REGIONS ! REGIONS is a comment
 C * Gas composition of each region; specify mole fraction of each gas
 C * No more than five columns at a time

Date: 12/31/98

A - 49

FAI/98-40, Rev. 1

```

JUNCTIONS 3 1 3 Junctions
* 1) MCO bottom to MCO middle, 1->2
* 2) MCO middle to MCO top, 2->3
* 3) MCO top to Outlet Volume, 1->5 (deactivated)

* SYNTAX:
* JTYVP Junction Type: 1 = Normal, 2 = HEPA, 3 = Cover
* IR1 Upstream Region
* IR2 Downstream Region
* AJN Area (m^2)
* PHFEA Bypass area for HEPA junction (m^2)
* MCOV HEPA Filter Failure Pressure (Pa)
* MCOV Cover Area (m^2)
* MCOV Cover Height (m)
* IR2 Elevation w/ floor of IR1 opening (m)
* IR2 IR2
* CJN Loss coefficient multiplies 0.5*theta^2
* ITHORIZ Orientation: 1 = horizontal, 0 = vertical
* XWJN Characteristic width, m
* XHJN Characteristic height, m
* XJN Characteristic length, m
* DFJN Decontamination factor
* N90 No. of 90 bends

PATHS 1 2 3
* IJTYVP 1 1 1
* IR1 3 3 1
* IR2 2 2 5
* ITHORIZ 1 1 1
* XWJN 0.61 0.61 2.54E-2
* XHJN 0.001 0.001 2.54E-2
* XJN 0.29 0.29 10
* IJN 1.2 1.2 10
* ZJN 0.0 0.0 12.65
* CJN 1.0 1.0 4.0
* DFJN 1.0 1.0 1.0
* N90 0 0 3

END PATHS ; PATHS is a comment.

END JUNCTIONS ; JUNCTIONS is a comment.

MCO
* MCO Major Keyword
* Keyword for general inputs
* -1, do oxidation of fuel/scrap
* -0, disable oxidation of fuel/scrap
* -1, do hydrating/dehydrating calculation
* -0, disable hydrating/dehydrating calculation
* -1, divert heat transfer to gas to gas
* -0, do not divert heat transfer to gas
* -1, do evaporation/condensation of liquid
* -0, do not evaporation/condensation of liquid
* -1, oxidation rate law, 0 - McGillivray/Ritchie
* -0, 1 - Pearce
* -1, de-entrainment of aerosol due to scrap basket
* -0, disable de-entrainment calculation

GENERAL
* IONDRN 1
* IHVD 0
* IDIVRT 0
* IEVAP 0
* ILAW 1
* IDENT 0

```

END HEAT SINKS ; HEAT SINKS is a comment

Date: 12/31/98

A - 50

FAI/98-40, Rev. 1

```

* PUMP IRPUM IROPUM ICONPM ITFRED WFPUMP WVFED TGFED TCONPM
* Definitions:
* IRPUM - Pump inlet region
* IROPUM - Pump outlet region
* ICONPM - Node to which the condensed steam is dumped for book-keeping
* ITFRED - If non-zero, override the TGFED with the designated region
* WFPUMP - Used to specified time-varying feed
* temperature. Used to specified time-varying feed
* Temperature Pump volumetric flowrate (m3/s)
* WVFED - Feed volumetric flowrate (m3/s)
* TGFED - Feed temperature (K)
* TCONPM - Condenser cooling coil temperature (K)
* 35 FT3/MIN * 1 MIN/60 SEC * 0.02832 M3/1 FT3 = 0.01652 M3/SEC
* PUMP IRPUM IROPUM ICONPM ITFRED WFPUMP WVFED TGFED TCONPM
* PUMP 1 5 0 1.652E-2 0.0 0.0 0.0
* Radiolysis parameters
* FRAD 1.0 ! multiplier for radiolysis
* FALPHA 0.197 ! alpha fractional heat load
* FBETA 0.486 ! beta fractional heat load
* FGAMMA 0.317 ! gamma fractional heat load
* QPHOTO 2.4E-6 ! heat production rate in MCO free water per gram
* ! heat of fuel loading
* ! heat of fuel loading
* ! GENERAL is a comment
* END GENERAL
* SOLAR_RAD
* ! pointers to heat sinks representing the cask wall and the top
* ! solar radiation impinges on these
* IHASK 42
* IHOP 44
* ! look-up table for solar radiation throughout a day (sec. vs. W/m2)
* OFFSET TIMOV 21600. ! offset by six hours
* EXTRAPOLATION_TIMOV PERIOD ! expect solar radiation cycle
* TIMOV 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
* 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
* 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
* 75600.0 79200.0 82800.0 86400.0
* RADGUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* END SOLAR_RAD
* FUEL_BSNT 2 ! Total number of fuel baskets
* ! Fuel Basket
* ! 1st Fuel Basket
* ! 1 2 3 4 5 6 7 8 9 10 11 12 13 14
* ! define the heat sink comprising the first fuel basket (must be
* ! in pairs, for inner and outer elements)
* ! IFLNS 0 ! define the adjacent center insert heat sink,

```

```

* do entrainment of sludge particle calculation
* -1, disable entrainment calculation
* -0, do decomposition of fuel oxide hydrate
* -1, do hydrate decomposition calculation
* -0, disable hydrate decomposition calculation
* -1, do nitriding calculation
* -0, disable nitriding calculation
* -1, do radiolysis calculation
* -0, disable radiolysis calculation
* -1, do average diameter calculation
* -0, disable average diameter calculation
* -1, define the cask heat sink
* -0, define the gap node (between MCO wall and the cask)
* -1, define the gap node (between the MCO wall and
* radiative/convective h.t. between the MCO wall and
* the cask is computed and some of the heat is
* to gas for stability
* ! gap distance between the MCO wall and the cask
* ! turn off the radiative heat transfer between the
* ! fuel and the lid/floor
* ! fully account for the radiative heat transfer
* ! sludge particle density (kg/m3)
* ! sludge specific area (m2/m3)
* ! sludge particle diameter (m)
* RHOSL 5000.
* SASL 1000.
* XOSL 1.8E-6
* Hydrate Model: two-step decomposition,
* input curves for ln p and ln K
* first step for x > XHVD2, second step for x < XHVD2
* 10 ! weight fraction of sludge being water is equivalent to 90 %
* of sludge being hydrated with 2 moles of
* water per mole of uranium oxide
* FHYSL 0.9 ! fraction of sludge that is hydrated
* XHNSL 2.0 ! stoichiometry number of hydrate, no. of moles of
* water per mole of uranium oxide (UO3.H2O)
* XHVD2 1.0 ! H2O/U ratio (stoich. number) to switch
* from second to third correlation
* XHVD3 0.5 ! H2O/U ratio (stoich. number) to switch
* from second to third correlation
* ADEY01 18.012 ! 'A' IN LN P = A + B/T FOR X > XHVD2
* BDEY01 -6775.E0 ! 'B' IN LN P = A + B/T FOR X > XHVD2
* ADEY02 19.076 ! 'A' IN LN P = A + B/T FOR X < XHVD2
* BDEY02 -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHVD2
* ADEY03 19.076 ! 'A' IN LN P = A + B/T FOR X < XHVD3
* BDEY03 -8312.E0 ! 'B' IN LN P = A + B/T FOR X < XHVD3
* ADEY11 -5.293E0 ! 'A' IN LN K = A + B/T FOR X > XHVD2
* BDEY11 -25.94E0 ! 'B' IN LN K = A + B/T FOR X > XHVD2
* ADEY12 -25.94E0 ! 'A' IN LN K = A + B/T FOR X < XHVD2
* BDEY12 -25.46E0 ! 'B' IN LN K = A + B/T FOR X < XHVD2
* ADEY13 -5.293E0 ! 'A' IN LN K = A + B/T FOR X < XHVD3
* BDEY13 -25.46E0 ! 'B' IN LN K = A + B/T FOR X < XHVD3
* DHY11 2.8656 ! Decomposition enthalpy J/kg H2O: 1st step
* DHY12 3.7086 ! Decomposition enthalpy J/kg H2O: 2nd step
* DHY13 3.7086 ! Decomposition enthalpy J/kg H2O: 3rd step
* FPROY 1.0 ! hydrate production rate law multiplier
* FCONY 1.0 ! hydrate consumption rate law multiplier
* FNTRI 1.0 ! nitriding rate law multiplier
* PUMP, FEED, AND CONDENSER MODELS
* Syntax:

```

A - 51

A.11 Entrainment Validation

```

* IHSCC 31 1 ring 1, theta
32 33 1 ring 2, theta
34 35 1 ring 3 & 4, radial
37 36 1 ring 6 & 5, radial
38 39 1 ring 11 & 12, radial

* ICSINS 0 1 define the adjacent center insert heat sink,
1 0 for no insert
ISCIN 41 1 define copper fin heat sink
ISCHCO 40 1 define the adjacent MCO wall heat sink
ISCLID 44 1 define the lid or floor heat sink to which the
scrap
1 radiate to

* porosity of the scrap for each heat sink in the order read in
(31, 32, 33, 34, ..)
PFOROS 0.45 0.45 0.45 0.45 0.6 0.6 0.6 0.6 0.6
characteristic size for each scrap heat sink in the order read in (m)
XSCGRP 0.00635 0.00635 0.00635 0.00635 0.00635
0.0234 0.0234 0.0234 0.0234 0.0234
XSCBVK 0.1491 0.1491 0.1491 0.1491 0.1491
XISCBK 0.691 0.691 0.691 0.691 0.691

* exposed surface area available for oxidation
per unit volume of scrap (1/m) for
each scrap basket heat sink in the order read in
Example:
6 m^2 bounding oxidation area: 6/0.17491 = 34.30 m^2
10 m^2 fine oxidation area: 10/0.01756 = 569.48 m^2/m^3
5.4 m^2 coarse oxidation area: 5.4/0.15734 = 34.32 m^2/m^3

* AVXSCC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
FOXSC 10 0.0 1 multiplier for AVXSCC on the exposed surface (m)
XSCXCO 0.0 1 initial oxide thickness on the exposed surface (m)

* FSCYBD 0.0 0 fraction of oxide which is hydride
1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
* 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
* MWSCCO 8.576 8.576 8.576 8.576 8.576 8.576 8.576 8.576
initial amount (kg) of water per unit bulk volume

* FWSGIO 0.0 1 (m^3) of scrap
1 on the outer surface of the insert
1 (per unit area, m^2)
1 on the inner surface of the MCO wall
FWSMCO 0.0 1 (per unit area, m^2) surface area
FWSMCC 0.1 1 wetted fraction of MCO wall
FWSMCH 1.0 1 wetted fraction of MCO wall
XSCINS 0.01 1 gap distance between the insert and scrap basket
1/4" gap for scrap basket and mco wall
XSCXCO 0.00635 1 gap distance between scrap basket and MCO wall
HSLSC 55.0 1 mass of sludge particles (kg) in the scrap basket
END IHSCC for 1st scrap basket
END SCRAP_BST
END MCO

```

A.11 Entrainment Validation

```

*****
MCO ENTRAINMENT CASE
*****
* FUEL BASKETS AND SCRAP BASKET
* INITIALLY, 11.355 (150) PSIG, 75 C, N2 FILLED
* BLOWDOWN THROUGH A 1 INCH VENT, FUEL AND SCRAP
* ACTIVATE ENTRAINMENT MODEL IENTR=1
*****
CONTROL 1 Major keyword group
*****
TITLE 1 Keyword; next line is title, title can be any length
MCO BLOWDOWN: N2 FILL, 150 PSIG, 75 C, 1 INCH VENT, FUEL AND SCRAP
END TITLE: Anything after END is a comment
*****
TIMING 1 Keyword
1 START TIME, >0 FOR RESTART RUN
1 RESTART FILE IS READ FROM HANSF.RER
1 END TIME (Seconds)
1 MIN TIMESTEP (Seconds)
1 MAX TIMESTEP (Seconds)
1 PRINT INTERVAL (Seconds)
1 MIN LOGINTERVAL (Seconds)
1 MIN LOGINTERVAL WITHOUT PLOT (Seconds)
1 RESTART INTERVAL (Seconds)
1 FRACTIONAL CHANGE IN T AND P
1 FRACTIONAL CHANGE IN AEROSOL MASS
1 FRACTIONAL CHANGE FOR PLOTTING
END TIMING 1 TIMING is a comment.
*****
PLOT 1 Keyword for plotting section
1 Plotting syntax:
* PRESSURE n rlist - Pressure, Pa
* GAS-T n rlist - Gas Temperature, K
* HS-TI n rlist - Heat Sink Temperature - Inner Surface, K
* HS-TO n rlist - Heat Sink Temperature - Outer Surface, K
* HS-TA n rlist - Heat Sink Temperature - Average, K
* GAS-MOL n rlist - Gas Molar Flowrate, kg/s
* GAS-WX n rlist - Mass Flowrate, kg/s
* GAS-WX n rlist - Counter-Current Mass Flowrate, kg/s
* GASNAME n rlist - Gas Name
* GAS-RH GASNAME n rlist - Gas Relative Humidity
* GAS-MASS GASNAME n rlist - Gas Mass (Species), kg
* AER-MASS GASNAME n rlist - Aerosol Mass (Species), kg
* MASS GASNAME n rlist - Total Mass (Species), kg
* LIQ-MASS GASNAME n rlist - Deposited Mass (Species), kg
* Pressure, Gas Temperature, and total aerosol mass require a region
* list

```

Date:

```
* Heat sink Temperatures need a heat sink number list
*
* Flowrates need a junction number list
*
* Gas concentration, relative humidity, individual species gas mass,
* individual species aerosol mass, total (gas+aerosol) individual
* species mass, and individual species deposited liquid mass require
* a region and gas name
*
PRESSURE      1   1           ! Pressure in MCO
AER-MASS     PUOZH2    2   1   3
PUOZOH2      1   1
LIQ-MASS     PUOZOH2    1   1
END PLOT      ! PLOT is a comment
*
ACTIVE MODELS ! Junction flow model
! Keyword; MODELS is a comment; 1 = on, 0 = off
JUNC         1   ! Junction flow model
ICFELW       0   ! Counter-current flow model
IHTHINK       1   ! Heat sinks
ICNDS        0   ! Condensation
IASD         1   ! Aerosol Sedimentation
IAESG        1   ! Aerosol Scavenging
TALCAN       0   ! Fog formation
ISRC         0   ! User-defined sources
IMCO         1   ! MCO models
ISENS        0   ! Sensitivity runs
END ACTIVE MODELS ! ACTIVE MODELS is a comment
*
SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
ENTER: TIME, TEMP, FLOWRATES, POWER
SYNTAX EXAMPLE:
* SOURCES 2 1 GASES 2
* STEAM HYDROGEN
* 0 300 1.E-3 1.E-3 0.E0
* 10 300 1.E-3 1.E-3 0.E0
END REGION
* REGION -1 GASES 1
* NAZO 300.0 4.44E-1 0.E0
* 10, 300.0 4.44E-1 0.E0
* 900, 300.0 4.44E-1 0.E0
* 901, 300.0 0.E0 0.E0
* 1.E5 300.0 0.E0 0.E0
END REGION
* END SOURCE
* END CONTROL ! End of CONTROL keyword group
*
VOLUMES      3   ! total number of control volumes
```


Date: 12/31/98[illegible]

IDENT	0	-1, de-entrainment of aerosol due to scrap basket
IENR	1	-1, 0, dis-entrainment calculation -1, 0, dis-entrainment of sludge particle calculation -1, 0, dis-entrainment calculation
IHYDRA	0	-1, 0, decomposition of fuel oxide hydrate -1, 0, dis-able hydrate decomposition calculation
INITRI	0	-1, 0, nitriding calculation -1, 0, dis-able nitriding calculation
IRADIO	0	-1, 0, radiolytic analysis calculation -1, 0, dis-able radiolytic analysis calculation
KHMO	5, E-5	-1, define diameter of hydride particle (m)
KUSCK	16	-1, define the gap heat sink
IRGAP	2	-1, define the gap node (between MCO wall and the cask) -1, radiative/convective h.t. between the MCO wall and the cask is computed and some of the heat is diverted
XGPCSK	0.001	-1, to gas for stability
PHILLID	0.0	-1, gap film coefficient between the MCO wall and the cask -1, 0, turn off the radiative heat transfer between the gap film/scrap and the lid/floor
RHOSL	5000.	-1, fully account for the radiative heat transfer sludge particle density (kg/m ³)
SASL	1000.	-1, sludge specific area (m ² /m ³)
XDSEL	1.E-6	-1, sludge particle diameter (m)
* * *		Hydrate Model; two-step decomposition,
* * *		hydrate model for ln p and ln K
* * *		first step for x > XHYD2, second step for x < XHYD2
* * *		10 % weight fraction of sludge being water is equivalent to 90 % of sludge being hydrated with 2 moles of water per mole of uranium oxide
FHWSL	0.9	-1, fraction of sludge that is hydrated
XHWSL	2.0	-1, stoichiometry number of hydrate: no. of moles of water per mole of uranium oxide (UO3.H2O)
XHYD2	1.0	-1, H2O/U ratio (stoich. number) to switch from first to second correlation
XHYD3	0.5	-1, H2O/U ratio (stoich. number) to switch from second to third correlation
AHTEQ1	19.012	-1, 'A' IN LN P = - A + B/T FOR X > XHYD2
BHEQ2	-17.850	-1, 'B' IN LN P = - A + B/T FOR X > XHYD2
CHEQ3	19.076	-1, 'C' IN LN P = - A + B/T FOR X < XHYD2
BHEQ2	-8312.1E0	-1, 'B' IN LN P = - A + B/T FOR X < XHYD2
AHTEQ3	19.076	-1, 'A' IN LN P = - A + B/T FOR X < XHYD2
BHEQ3	-8312.1E0	-1, 'B' IN LN P = - A + B/T FOR X < XHYD3
ADHENY1	-5.29580	-1, 'A' IN LN K = - A + B/T FOR X < XHYD2
BDEHY1	-2546.2E0	-1, 'B' IN LN K = - A + B/T FOR X < XHYD2
ADHENY2	-5.29580	-1, 'A' IN LN K = - A + B/T FOR X < XHYD2
BDEHY2	-2546.2E0	-1, 'B' IN LN K = - A + B/T FOR X < XHYD2
ADHENY3	-5.29580	-1, 'A' IN LN K = - A + B/T FOR X < XHYD3
BDEHY3	-2546.2E0	-1, 'B' IN LN K = - A + B/T FOR X < XHYD3
DERTH1	2.7865E6	-1, Decomposition enthalpy J/kg H2O: 1st step
DERTH2	3.708E6	-1, Decomposition enthalpy J/kg H2O: 2nd step
DERTH3	3.708E6	-1, Decomposition enthalpy J/kg H2O: 3rd step
PFRHY	2.708E6	-1, hydrate production rate law multiplier
PCOHNY	1.0	-1, hydrate consumption rate law multiplier
FNTRI	1.0	-1, nitriding rate law multiplier

A - 55

HEAT SINKS ! HEAT SINKS is a comment

FUNCTIONS 1 ! 3 Junctions

2000-01-01

- * 1) MCO bottom to MCO top, 2->1
- * 2) MCO middle to MCO top, 2->1

* 3) MCO top to outlet volume, 1-23 (deactivated),

* syntax:

```

* IJTYPE      Junction Type: 1 = Normal, 2 = HEFA, 3
* IJTYPE      Junction Type: 1 = Normal, 2 = HEFA, 3

```

* TR1 Upstream Region

* TR2 Downstream Region

* AJN
Area (m^2)
Number area for HEPA function (m^2)

* PHEPA HEPA Filter Failure Pressure (Pa)

* ACOV
Cover Area (m²)
Cover Height (W)

Station	Elevation wrt floor of IRI opening (m)
21JN	1.0

* 22JN γ coefficient multiplies $0.5 \cdot \rho \cdot h \cdot v^2$

* ITHORZ Orientation: 1 = horizontal, 0 = vertical

* XWJN Characteristic width, in characteristic height. M

* XLJN Characteristic length, m

* * * * *	DEFJN	Decontamination Factor
* * * * *	N90	No. of 90 bends

PATHS

ИЖТҮР 1

IR1	IR2	IR3
1	1	1
2	2	2
3	3	3
4	4	4
5	5	5
6	6	6
7	7	7
8	8	8
9	9	9
10	10	10
11	11	11
12	12	12
13	13	13
14	14	14
15	15	15
16	16	16
17	17	17
18	18	18
19	19	19
20	20	20
21	21	21
22	22	22
23	23	23
24	24	24
25	25	25
26	26	26
27	27	27
28	28	28
29	29	29
30	30	30
31	31	31
32	32	32
 
84	84	84
85	85	85
86	86	86
87	87	87
88	88	88
89	89	89
90	90	90
91	91	91
92	92	92
93	93	93
94	94	94
95	95	95
96	96	96
97	97	97
98	98	98
99	99	99
100	100	100

THORIZ 0 5 5 0

2.54E-2

XLJN 0.100 5.07E-4

3.95
Z1JN

22JN 3.95

DEFN 1.0

N90 3
one name, name is a comment.

— 1 —

END JUNCTIONS I JUNCTIONS IS A COMMENT:

MCO ! MCO Major Keyword

***** Requested for general inbuds

TOXPTN	1
I =1, do oxidation of fuel/scra	

—

```

I=0, disable hydriding/dehydriding

```

IDIVRT 1 1 =1, divert heat transfer to 9

TEVAP	0
! =1, do evaporation/condensation	

```
! =0, do not do evaporation/condensation
! condensation rate law 0 = McGill
```

WTWTT
1 - pearc

—
\$
\$
\$
\$
—

FAI/98-40, Rev. 1

```

* PUMP, FEED, AND CONDENSER MODELS
* SYNTAX:
* PUMP IRPUM IROPUM ICONPM ITFED WVPUMP WVFED TGFED TCNPM
Definitions:
* IRPUM - Pump inlet region
* IROPUM - Pump outlet region
* ICONPM - Node to which the condensed steam is dumped for book-keeping
* ITFED - If non-zero, overrides TGFED with the designated region
* TGFED - Temperature. Used to specified time-varying feed
* TCNPM - Condenser cooling coil temperature (K)
* WVPUMP - Pump volumetric flowrate (m3/s)
* WVFED - Feed volumetric flowrate (m3/s)
* TFEED - Feed temperature (K)
* TCOND - Condenser cooling coil temperature (K)
* 35 FT3/MIN * 1 MIN/60 SEC * 0.02832 M3/A FT3 = 0.01652 M3/SEC
* PUMP IRPUM IROPUM ICONPM ITFED WVPUMP WVFED TGFED TCNPM
* PUMP 1 5 0 1.652E-2 0.0 0.0 0.0
* Radiolysis parameters
* FRAD 1.0 ! multiplier for radiolysis
* FALPHA 0.197 ! alpha fractional heat load
* FBETA 0.486 ! beta fractional heat load
* FGAMMA 0.317 ! gamma fractional heat load
* QPHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
! PARTIAL OF FUEL
! GENERAL is a comment
END GENERAL
* SOLAR_RAD
* pointers to heat sinks representing the cask wall and the top
* solar radiation impinges on these
* IHCSK 42
* IHPOP 44
* look-up table for solar radiation throughout a day (sec .vs. W/m2)
* OFFSET TIMDAY 21600. ! offset by six hours
* EXTRAPOLATION TIMDAY PERIOD ! repeat the diurnal cycle
* TIMDAY 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
* 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
* 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
* 75600.0 79200.0 82800.0 86400.0
* RAD SUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* END SOLAR_RAD
* END FUEL_BSKT
* FUEL_BSKT 1 ! Total number of fuel baskets
* 1st Fuel Basket
* IHSELF 1 2 3 4 5 6 7 8 9 10 11 12 13 14
* define the heat sinks comprising the first fuel basket (must be
* in pairs, for inner and outer elements)

```

```

* IFINS 0 ! define the adjacent center insert heat sink,
* 0 for no insert, 1 for adjacent MCO wall heat sink
* IFMCO 15 ! define the adjacent MCO wall heat sink
* IFLLID 0 ! define the lid or floor heat sink to which the fuel
* radiate to
* AFUEL 0.131 ! flow area in the basket
* fraction of geometric area exposed for oxidation
* " area available for oxidation/total heat sink area
* FMOXEL 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
* FMOXEL 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000
* FOX 0.00000 0.1 ! multiplier for FMOXEL
* XFLOXO 1.8-4 ! initial oxide (oxidohydrate) thickness
* ! (to be applied to exposed area)
* FXHYDRO 0.0 ! fraction of initial oxide which is hydrate
* initial amount (kg) of water per geometric surface area (m2) of fuel
* FWEL0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
* 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
* FWEL10 0.0 ! on the outer surface of the insert
* 0.0 ! on the inner surface of the MCO wall
* FMOXEL 0.0 ! wetted fraction of fuel surface
* FMOXEL 0.1 ! wetted fraction of MCO wall
* FMOXEL 1.0 ! wetted fraction of MCO wall
* MSLEFL 87.6 ! mass of sludge particles (kg) in the fuel basket
* view factor matrix between the insert,
* outer surface of outer fuel basket,
* and the MCO wall, therefore, the dimension of the square matrix is
* number of fuel rods+1. If there is no insert, number of fuel
* rods+1.
* FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000 0.000
* 0.316 0.027 0.316 0.158 0.018 0.009 0.000 0.000 0.000
* 0.176 0.316 0.000 0.167 0.158 0.009 0.000 0.000 0.000
* 0.009 0.316 0.334 0.158 0.018 0.018 0.158 0.107
* 0.000 0.158 0.158 0.158 0.018 0.018 0.158 0.208
* 0.000 0.009 0.018 0.167 0.316 0.316 0.048 0.558
* 0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
* gap distance for micro-convection calculation
* XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
* 0.037 0.000 0.037 0.037 0.056 0.056 0.056 0.000
* 0.037 0.037 0.000 0.037 0.037 0.037 0.037 0.090
* 0.056 0.037 0.037 0.000 0.000 0.056 0.037 0.090
* 0.000 0.056 0.037 0.037 0.056 0.000 0.037 0.056
* 0.000 0.056 0.037 0.037 0.037 0.037 0.037 0.043
* 0.000 0.000 0.037 0.037 0.037 0.037 0.037 0.000
* 0.000 0.000 0.000 0.090 0.090 0.056 0.043 0.000
* END IHSELF for 1st fuel basket
* END FUEL_BSKT
* SCRAP_BSKT 1 ! Total number of scrap baskets
* IHSSC 20 21 22 23 24 ! ring 1, theta

```

```

* - Fuel is initialized to 150 C and the MCO wall temperature is
  fixed to 150 C
* - Bottled-up MCO
*****
CONTROL ! Major keyword group
-----
*
* TITLE ! Keyword; next line is title, title can be any length
DEHYD - Dehydration Model Validation
END TITLE ! Anything after END is a comment
*
* TIMING ! Keyword
TSTART 0.
TSTOP 100000.
DTMIN 0.01
DTMAX 5.0
PRINT 1000.
PRINT 1000.
PLTMAX 1000.
PLTMIN 1000.
DTEST 10000.
RESTART INTERVAL (Seconds)
FTECH 0.005
FASCH 0.005
FPELCH 0.03
END TIMING ! TIMING is a comment.
*
* PLOTTING ! Keyword for plotting section
* Plotting syntax:
* PRESSURE n rlist - Pressure, Pa
* GAS-T n rlist - Gas Temperature, K
* HS-TI n rlist - Heat Sink Temperature - Inner Surface, K
* HS-TO n rlist - Heat Sink Temperature - Outer Surface, K
* HS-TA n rlist - Heat Sink Temperature - Average, K
* GASCOL n rlist - Gas Collection (kg/s), kg
* GAS-WX n rlist - CounterCurrent Mass Flowrate, kg/s
* GAS-X GASNAME n rlist - Gas Mole Fraction
* GAS-RH GASNAME n rlist - Gas Relative Humidity
* GAS-MASS GASNAME n rlist - Gas Mass (Species), kg
* AER-MASS GASNAME n rlist - Aerosol Mass (Species), kg
* MASS GASNAME n rlist - Total Mass (Species), kg
* LIQ-MASS - GASNAME n rlist - Deposited Mass (Species), kg
* Pressure, Gas Temperature, and total aerosol mass require a region
  list
* Heat Sink Temperatures need a heat sink number list
* Flowrates need a junction number list
* Gas concentration, relative humidity, individual species gas mass,
  individual species aerosol mass, total (gas+aerosol) individual
  species mass, and individual species deposited liquid mass require
  a list

```

A - 57

FAU/98-40, Rev. 1

Date: 12/31/98

A.12 Hydrate Decomposition Validation

```

*****
* Dehydration Model Validation - DEHYD.DAT
*
* UNLESS OTHERWISE NOTED, MKS UNITS
*
* - 1 TIER OF SCRAP BASKET
* - 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
*
* - Fuel corrosion, evaporation/condensation, hydrating and nitrating
  were turned off

```

```

ISCINS 0 ! define the adjacent center insert heat sink,
ISCFIN 24 ! 0 for no insert
ISCHCO 25 ! define copper fin heat sink
ISCHCB 0 ! define the adjacent MCO wall heat sink
ISCHCB 0 ! define the lid or floor heat sink to which the
  scrap
* porosity of the scrap for each heat sink in the order read in
*
* PFOROS 0.50 0.50 0.50 0.50
* characteristic size for each scrap heat sink in the order read in (m)
* XDCRCP 0.006 0.006 0.006 0.006
* XRSCHBK 0.2920 ! radius of scrap basket (m)
* XRSCHBK 0.663 ! height of scrap basket (m)
*
* exposed surface area available for oxidation
* PEXPOS 0.0 ! (m^2) for
* PEXPOS 0.0 ! (m^2) for
* Example:
* 6 m^2 bounding oxidation area: 6/0.17491 = 34.30 m^2
* 10 m^2 fine oxidation area: 10/0.01756 = 569.48 m^2/m^3
* 5.4 m^2 coarse oxidation area: 5.4/0.15734 = 34.32 m^2/m^3
*
* AVOSXC 300. 300. 300. 300.
* AVOSXC 300. 300. 300. 300.
* AVOSXC 1.0 ! initial oxide thickness on the exposed surface (m)
* AVOSXC 1.0 ! 1.0
* FSCYD 0.1 ! fraction of oxide which is hydride
* MVNSCO 0.
*
* FWSCIO 0.0 ! (m^3) of scrap
* ! on the outer surface of the insert
* ! (per unit area, m^2)
* FWSCMO 0.0 ! (per unit area, m^2)
* ! wetted fraction of the MCO wall
* FWSC 0.1 ! wetted fraction of MCO wall
* FAWSCM 1.0 ! gap distance between the insert and scrap basket
* XSCINS 0.01 ! 1/4" gap for scrap basket and mco wall
* XSCMCO 0.00635 ! gap distance between scrap basket and MCO wall
* MSLSC 55.0 ! mass of sludge particles (kg) in the scrap basket
* END THSCC for 1st scrap basket
* END SCRAP_BSKT
* END MCO

```


Date: 12/31/98

A - 59

FAI/98-40, Rev. 1

```

* No more than five columns at a time, so continue with 6 & 7
* AEROSOLS 6 7
* STEAM 0.0
* END AEROSOLS ! AEROSOLS is a comment
*
* OPTIONAL TEMPERATURE AND PRESSURE CONTROL
* MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
* TEMPS TEMPERATURE LOOK-UP TABLE
* SYNTAX:
*   OFFSET TIMETG
*   EXTRAPOLATION TIMETG
*   TIMEG IREG TIME1, TIME2...TIMELAST
*   TGEIX IREG TIME1, TIME2...TIMELAST
*   LINEAR INTERPOLATION BETWEEN VALUES
*
* SIMILAR SYNTAX FOR PRESSURE:
*   OFFSET TIMETG
*   EXTRAPOLATION TIMETG
*   TIMEP IREG PRES1, PRES2...PRESSURES ARE IN PA!!!
*   PREIX IREG PRES1, PRES2...PRESSURES ARE IN PA!!!
*
* OFFSET TIMETG- OFFSET TIME; ENTER LOOKUP TABLE WITH
*   TIME-OFFSET TIMETG
*   TIME-OFFSET TIMETG
*   EXTRAPOLATION_TIMETG= LAST TO USE LAST VALUE IN THE TABLE,
*   = EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
*   = PERIOD TO WRAP AROUND.
*
* OFFSET TIMETG
*   50.
*   EXTRAPOLATION TIMETG LAST
*   TIMEG 1 0.0 100 400.
*   TGEIX 1 293.15 393.15 473.15
*
* CONTROL MCO BOUNDARY P, 30.
*   OFFSET TIMETG
*   EXTRAPOLATION TIMETG EXTRAP
*   TIMEP 1 0.0 100. 200.
*   PREIX 1 1.E5 1.2E5 1.4E5
*
* END VOLUMES ! VOLUMES is a comment
*
* Major keyword-----
* HEAT SINKS 44 ! Total number of heat sinks
*
* * decay power based on 835 W per MCO.
* * No more than 5 columns at a time,
* * Repeat the following structure,
* * SINKS
* *
* *
* *
* * END
*
* Syntax:
* * IGEOM 1 for plane, 0 or 2 for cylinder
* * RHO Density (kg/m3)
* * KHS Thermal conductivity (W/m/K)
* * CPHS Specific Heat (J/kg/K)
* * QV Volumetric Heat Generation (W/m3)

```

```

* XRI Inner Radius (m)
* XRO Outer Radius (m); for plane wall, thickness = XRO-XRI
* AHS One-sided heat sink area (m2)
* TINIT Initial inside surface temperature (C)
* TOUTIT Initial outside surface temperature (C)
* INSLAB Number of slabs; 3 is minimum
* IREGI Region index for inner surface or 0 (insulated)
* or -1 for constant temperature
* TINS Region index for inner surface when IREGI = -1 (C)
* IREGO Region index for outer surface or 0 (insulated)
* or -1 for constant temperature
* TOHS Region surface temperature when IREGO = -1 (C)
* XHS Characteristic length for natural convection (m)
* EHSI Emissivity of inner surface
* EHSO Emissivity of outer surface
*
* Fuel Basket #1 heat sinks 1 through 15
* SINKS 1 2 3 4 5
*
* IGEOM 1
* RHO 18768. 18768. 18768. 18768. 18768.
* KHS 26.9 26.9 26.9 26.9 26.9
* CPHS 122.67 122.67 122.67 122.67 122.67
* QV 0.0 0.0 0.0 0.0 0.0
* XRI 0.0 0.0 0.0 0.0 0.0
* XRO 0.0102 0.0102 0.0102 0.0102 0.0102
* AHS 0.557 0.557 0.557 0.557 0.557
* IREGI 150.00 150.00 150.00 150.00 150.00
* IREGO 150.00 150.00 150.00 150.00 150.00
* TOHS 150.00 150.00 150.00 150.00 150.00
* EHSI 0.7 0.7 0.7 0.7 0.7
* EHSO 0.7 0.7 0.7 0.7 0.7
*
* END
*
* SINKS 6 7 8 9 10
*
* IGEOM 1
* RHO 18768. 18768. 18768. 18768. 18768.
* KHS 26.9 26.9 26.9 26.9 26.9
* CPHS 122.67 122.67 122.67 122.67 122.67
* QV 0.0 0.0 0.0 0.0 0.0
* XRI 0.0 0.0 0.0 0.0 0.0
* XRO 0.0092 0.0102 0.0102 0.0092 0.0092
* AHS 1.310 1.310 1.310 1.310 1.310
* IREGI 150.00 150.00 150.00 150.00 150.00
* IREGO 150.00 150.00 150.00 150.00 150.00
* TOHS 150.00 150.00 150.00 150.00 150.00
* EHSI 0.7 0.7 0.7 0.7 0.7
* EHSO 0.7 0.7 0.7 0.7 0.7
*
* END
*
* SINKS 11 12 13 14 15
*
* IGEOM 1
* RHO 18768. 18768. 18768. 18768. 18768.
* KHS 26.9 26.9 26.9 26.9 26.9
* CPHS 122.67 122.67 122.67 122.67 122.67
* QV 0.0 0.0 0.0 0.0 0.0
* XRI 0.0 0.0 0.0 0.0 0.0
* XRO 0.0102 0.0102 0.0102 0.0102 0.0102
* AHS 0.557 0.557 0.557 0.557 0.557
* IREGI 150.00 150.00 150.00 150.00 150.00
* IREGO 150.00 150.00 150.00 150.00 150.00
* TOHS 150.00 150.00 150.00 150.00 150.00
* EHSI 0.7 0.7 0.7 0.7 0.7
* EHSO 0.7 0.7 0.7 0.7 0.7
*
* END

```



```

* END GENERAL
! per MTU of fuel loading
! GENERAL is a comment

* SOLAR_RAD
* pointers to heat sinks representing the cask wall and the top
* solar radiation impinges on these
*
* IHCASK 42
* IHTOP 44
*
* look-up table for solar radiation throughout a day (sec. vs. W/m^2)
*
* OFFSET TIMDAY 21600. ! offset by six hours
* EXTRAPOLATION TIMDAY PERIOD ! repeat the diurnal cycle
* TIMDAY 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
* 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
* 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
* 75600.0 79200.0 82800.0 86400.0
* RAD SUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
*
* END SOLAR_RAD
*
* FUEL_BSKT 2 ! Total number of fuel baskets
*
* 1st Fuel Basket
*
* IHSFL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
! define the heat sinks comprising the first fuel basket (must be
! in pairs, for inner and outer elements)
*
* IFLINS 0 ! define the adjacent center insert heat sink,
! for no insert
* IFLMCO 15 ! define the adjacent MCO wall heat sink
* IFLID 0 ! define the lid or floor heat sink to which the fuel
! radiate to
* AFUFL 0.131 ! flow area in the basket
*
* fraction of geometric area exposed for oxidation
*
* area available for oxidation/total heat sink area
*
* 6.8 m^2 / (2*33.6 m^2) = 0.10119
* FAOXFL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
* 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
* FOX 10 0.0 ! multiplier for FAOXFL
* FXLOX 0.0 ! initial oxide (oxide-hydride) thickness
! (to be applied to exposed area)
* FXHDO 0.0 ! fraction of initial oxide which is hydride
*
* initial amount (kg) of water per geometric surface area (m^2) of fuel
* 24 kg / (2*33.6 m^2) = 0.3571
* 8.6/2/16.8 = 0.256 kg/m^2 (per side)
* FWFLD 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* FWFLTO 0.0 ! on the outer surface of the insert
* FWFLIO 0.0 ! on the inner surface of the MCO wall
* FWFLMO 0.1 ! wetted fraction of fuel surface

```

```

FAMEFLM 1.0 ! wetted fraction of MCO wall
MSLFL 45.0 ! mass of sludge particles (kg) in the fuel basket
! 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,
* outer surface and outer fuel elements,
* for the MCO wall. Therefore, the dimension of the square matrix is
* 1-number of fuel rods+1. If there is no insert, number of fuel
* rods+1.
*
* FVIEW 0.492 0.316 0.176 0.099 0.000 0.000 0.000 0.000 0.000
* 0.316 0.027 0.316 0.158 0.018 0.009 0.000 0.000 0.000
* 0.176 0.316 0.000 0.167 0.158 0.018 0.000 0.000 0.000
* 0.018 0.316 0.334 0.158 0.000 0.018 0.158 0.107
* 0.000 0.009 0.000 0.158 0.018 0.000 0.158 0.208
* 0.000 0.000 0.000 0.018 0.167 0.316 0.316 0.048 0.558
* 0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
*
* gap distance for micro-convection calculation
*
* XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
* 0.037 0.000 0.037 0.037 0.056 0.000 0.000 0.000
* 0.037 0.037 0.037 0.037 0.037 0.000 0.037 0.037 0.090
* 0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.037 0.056
* 0.000 0.056 0.000 0.037 0.037 0.056 0.000 0.037 0.056
* 0.000 0.000 0.037 0.037 0.037 0.037 0.000 0.043
* 0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.043 0.000
*
* END IHSFL for 1st fuel basket
*
* 2nd Fuel Basket
*
* heat sink pairs for second fuel basket
*
* IHSFL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
! define the adjacent center insert heat sink,
! for no insert
* IFLMCO 30 ! define the adjacent MCO wall heat sink
* IFLID 43 ! define the lid or floor heat sink to which the fuel
! radiate to
* AFUFL 0.131 ! flow area in the basket,
*
* fraction of geometric area exposed for oxidation
* 6.8 m^2 / (2*33.6 m^2) = 0.10119
* FAOXFL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
* 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
* FOX 10 0.0 ! multiplier for FAOXFL
* FXLOX 0.0 ! initial oxide (oxide-hydride) thickness
! (to be applied to exposed area)
* FXHDO 0.0 ! fraction of initial oxide which is hydride
*
* initial amount (kg) of water per geometric surface area (m^2) of fuel
* 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* FWFLIO 0.0 ! on the outer surface of the insert
* FWFLMO 0.0 ! on the inner surface of the MCO wall
* FWFLMO 0.4545 ! on the inner surface of the MCO wall

```

```

* each scrap basket heat sink in the order read in
* Example:
* 6 m2 bounding oxidation area: 6/0.17491 = 34.30 m2
* 10 m2 bounding oxidation area: 10/0.01756 = 569.48 m2/m3
* 5.4 m2 coarse oxidation area: 5.4/0.15734 = 34.32 m2/m3
*
* ANOXSC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
* FOXSC 10 0.0 ! multiplier for ANOXSC
* XSCOX0 0.0 ! initial oxide thickness on the exposed surface (m)
*
* FSCYHD 0.0 ! fraction of oxide which is hydride
* ! 1.5 kg of water to fill scrap basket; 1.5/0.17491 = 8.576 kg/m3
* MWNSC0 8.576 ! initial amount (kg) of water per unit bulk volume
* ! (m3) of scrap
* FMSCH0 0.0 ! on the outer surface of the insert
* ! (per unit area, m2)
* FMSCH0 0.0 ! on the inner surface of the MCO wall
* ! (per unit area, m2)
* FAWSC 0.1 ! wetted fraction of MCO wall surface area
* FAWSCM 1.0 ! wetted fraction of scrap basket and MCO wall
* XSCINS 0.01 ! gap, mm, between the insert and scrap basket
* XSCMCO 0.00635 ! gap distance between scrap basket and MCO wall
* ! (m)
* ! mass of sludge particles (kg) in the scrap basket
* ENHSSC for 1st scrap basket
* END SCRAP_BSKT
*
* END MCO

```

A.13 Fuel and Scrap Basket Heat Transfer Validation

```

***** SCRAP1.DAT - VALIDATION OF SCRAP BASKET MODEL WITHOUT CORROSION *****
*
* SCRAP INITIALLY AT 50 C
* a. FIN KEPT AT 50 C
* b. FIN KEPT AT 50 C
* c. H.T. TO GAS DISABLED
* d. OXIDATION MODEL DISABLED
* e. EVAPORATION MODEL DISABLED
* f. DEHYDRATION MODEL DISABLED
*
* - 1 TIER OF SCRAP BASKET
* - 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
*
*****
*
* CONTROL ! Major keyword group
*
*
* TITLE ! Keyword; next line is title, title can be any length
* SCRAP1.DAT VALIDATION OF SCRAP BASKET MODEL WITHOUT CORROSION
* END TITLE ! Anything after END is a comment
*

```

```

* view factor matrix between the insert,
* outer surface of outer fuel elements,
* and MCO wall. Therefore, the dimension of the square matrix is
* number of fuel rods*1. If there is no insert, number of fuel
* rods*1.
*
* FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
* 0.316 0.027 0.316 0.167 0.018 0.009 0.000 0.000
* 0.176 0.316 0.030 0.167 0.158 0.000 0.009 0.000
* 0.009 0.018 0.158 0.016 0.316 0.167 0.022
* 0.018 0.316 0.030 0.167 0.158 0.000 0.018 0.107
* 0.009 0.018 0.158 0.016 0.316 0.000 0.158 0.208
* 0.000 0.009 0.018 0.158 0.016 0.316 0.048 0.358
* 0.000 0.000 0.018 0.167 0.316 0.460 0.106
* 0.000 0.000 0.000 0.018 0.176 0.343
*
* gap distance for micro-convection calculation
*
* XGNP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
* 0.037 0.000 0.000 0.037 0.056 0.056 0.000 0.000
* 0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000
* 0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090
* 0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.090
* 0.000 0.056 0.000 0.037 0.056 0.000 0.037 0.043
* 0.000 0.000 0.037 0.037 0.037 0.037 0.037 0.043
* 0.000 0.000 0.000 0.090 0.090 0.090 0.036 0.043 0.000
*
* END INHSL for 2nd fuel basket
* END FUEL_BSKT
*
* SCRAP_BSKT 1 ! Total number of scrap baskets
*
* INHSC 31 ! ring 1, theta
* 32 33 ! ring 2, theta
* 34 35 ! ring 3 & 4, radial
* 37 36 ! ring 6 & 5, radial
* 38 39 ! ring 11 & 12, radial
*
* XSCINS 0 ! define the adjacent center insert heat sink,
* 0 for no insert
* XSCMCO 40 ! define copper fin heat sink
* INHSC 41 ! define the adjacent MCO wall heat sink
* INHSC 42 ! define the adjacent MCO wall heat sink
* INHSC 43 ! define the lid or floor heat sink to which the
* scrap
* INHSC 44 ! define the lid or floor heat sink to which the
* scrap
*
* porosity of the scrap for each heat sink in the order read in
* (31, 32, 33, 34, ...) 0.45 0.45 0.45 0.6 0.6 0.6 0.6
*
* FPOSOS 0.45 0.45 0.45 0.45 0.45 0.45 0.45 0.45
*
* characteristic area for each scrap heat sink in the order read in (m)
* XSCINS 0.00635 0.00635 0.00635 0.00635 0.00635 0.00635
* XSCMCO 0.0254 0.0254 0.0254 0.0254 0.0254 0.0254
* XSCBKT 0.2860 ! radius of scrap basket (m)
* XSCBKT 0.691 ! height of scrap basket (m)
*
* exposed surface area available for oxidation
* * per unit volume of scrap (1/m) for

```


A - 66

* SINKS	26	27	28	29	MCO WALL	50.00	50.00	50.00	50.00	50.00	50.00	50.00
* IGEOM	1	1	1	1	8000.	1	1	1	1	1	1	1
RHO	18768.	18768.	18768.	18768.	8000.	0.0	0.0	0.0	0.0	0.0	0.0	0.0
KHS	26.9	26.9	26.9	26.9	16.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	122.67	122.67	122.67	122.67	500.0	0.59	0.59	0.59	0.59	0.59	0.59	0.59
QV	2131.00	2131.00	2131.00	2131.00	0.0	0.7	0.7	0.7	0.7	0.7	0.7	0.7
XRI	0.0	0.0	0.0	0.0	0.0092	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XRO	0.0	0.0	0.0	0.0	0.0127	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AHS	0.0102	0.0092	0.0114	0.0127	2.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TIINIT	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00
TOINIT	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00	50.00
INSLAB	3	3	3	3	3	1	1	1	1	1	1	1
IREGI	3	3	3	3	3	8000.0	8000.0	8000.0	8000.0	8000.0	8000.0	8000.0
TIHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	3	3	3	3	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOHS	0.0	0.0	0.0	0.0	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XLHS	0.61	0.63	0.66	0.63	3.950	0.0	0.0	0.0	0.0	0.0	0.0	0.0
XHS	0.7	0.7	0.7	0.7	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
EHSD	0.7	0.7	0.7	0.7	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
END												
* scrap basket heat sinks 31 through 41												
* SINKS	R1-1	R2-2	R2-3	R3-4	R4-5							
	31	32	33	34	35							
* IGEOM	1	1	1	0	0							
RHO	18768.	18768.	18768.	18768.	18768.							
KHS	26.9	26.9	26.9	26.9	26.9							
CPHS	122.67	122.67	122.67	122.67	122.67							
QV	2131.00	2131.00	2131.00	2131.00	2131.00							
XRI	0.0	0.0	0.0	0.0	0.0							
XRO	0.02170	0.01423	0.01423	0.01423	0.07866							
AHS	0.10700	0.10700	0.10700	0.10700	0.30277							
TIINIT	50.00	50.00	50.00	50.00	50.00							
TOINIT	50.00	50.00	50.00	50.00	50.00							
INSLAB	5	5	5	5	5							
IREGI	1	1	1	1	1							
TIHS	0.0	0.0	0.0	0.0	0.0							
IREGO	1	1	1	1	1							
TOHS	0.0	0.0	0.0	0.0	0.0							
XLHS	0.69	0.69	0.69	0.69	0.69							
EHSD	0.7	0.7	0.7	0.7	0.7							
END												
* SINKS	R5-6	R6-7	R7-8	R8-9	FIN							
	36	37	38	39	40							
* IGEOM	0	0	0	0	1							
RHO	18768.	18768.	18768.	18768.	8954.0							
KHS	26.9	26.9	26.9	26.9	398.0							
CPHS	122.67	122.67	122.67	122.67	384.0							
QV	2131.00	2131.00	2131.00	2131.00	0.0							
XRI	0.09552	0.14389	0.14389	0.14389	0.00318							
XRO	0.52189	0.52189	0.52189	0.52189	0.26301							
TIINIT	50.00	50.00	50.00	50.00	50.00							

* USER CAN CONTROL HEAT SINK BOUNDARY TEMPERATURE
* SYNTAX: OFFSET_TIMES

A - 69

FAI/98-40. Rev. 1

[illegible]

A - 71

Date: 12/31/98

A - 73

FAI/98-40, Rev. 1

```

* Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
*
GASES      1      2      3      4      5
HELIUM      0.1      0.1      0.1      0.1      0.0
STEAM       0.0      0.0      0.0      0.0      0.010
OXYGEN      0.0      0.0      0.0      0.0      0.205
NITROGEN    0.9      0.9      0.9      0.9      0.0
END GASES   0.0      0.0      0.0      1.0      0.0
! GASES is a comment
* If there are more than five regions, continue here.
*
GASES      6      7
HELIUM      0.99      0.059
STEAM       0.11      0.069
OXYGEN      0.0      0.069
NITROGEN    0.0      0.7775
WATER       0.0      0.0
END GASES   ! GASES is a comment
* Aerosol concentration of each region (kg/m3)
* No more than five columns at a time
*
AEROSOLS    1      2      3      4      5
STEAM       0.0001      0.0      0.0      0.0      0.0
END AEROSOLS ! AEROSOLS is a comment
* No more than five columns at a time, so continue with 6 & 7
*
AEROSOLS    6      7
STEAM       0.0      0.0
END AEROSOLS ! AEROSOLS is a comment
* OPTIONAL TEMPERATURE AND PRESSURE CONTROL
* CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
* IMPOSE TEMPERATURE LOOK-UP TABLE
* SYNTAX:
* OFFSET TIMETG
* EXTRAPOLATION TIMETG
* TIMETG IREG TIME1, TIME2...TIMELAST
* TGRX IREG TIME1, TIME2...TIMELAST
* LINEAR INTERPOLATION BETWEEN VALUES
* SIMILAR SYNTAX FOR PRESSURE:
* OFFSET TIMETG
* EXTRAPOLATION TIMETG
* TIMETG IREG TIME1, TIME2...
* PREFIX IREG PRES1, PRES2...PRESSURES ARE IN PA!!!
* OFFSET TIMETG= OFFSET TIME; ENTER LOOKUP TABLE WITH
* TIME-OFFSET TIMETG= LAST TWO LAST VALUE IN THE TABLE.
* EXTRAPOLATION TIMETG= LAST TWO LAST VALUE IN THE TABLE.
* = PERIOD TO WRAP AROUND.
* OFFSET TIMETG LAST
* EXTRAPOLATION TIMETG 50.
* TIMETG 1 0.0 100.

```

```

ISRC 0 ! User-defined sources
IMCO 1 ! MCO models
ISENS 0 ! Sensitivity runs
END ACTIVE MODELS ! ACTIVE MODELS is a comment
*
C-----
C SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
C END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
C ENTER: TIME, TEMP, FLOWRATES, POWER
C SYNTAX EXAMPLE:
C REGION 1 GASES 2 !--- KEYWORD AND # SOURCE GROUPS
C STEAM HYDROGEN !--- REGION #, # GASES
C 0 300 1.E-3 1.E-3 0.E0 !--- GAS NAMES MUST BE ON NEXT LINE
C 10 300 1.E-3 1.E-3 0.E0
C END REGION
C REGION -1 GASES 1
C MCO 300.0 4.44E-1 0.E0
C 0 300.0 4.44E-1 0.E0
C 10 300.0 4.44E-1 0.E0
C 900. 300.0 4.44E-1 0.E0
C 901. 300.0 0.E0 0.E0
C 1.E5 300.0 0.E0 0.E0
C END REGION
C !--- ENDS A REGION SOURCE
C !--- ENDS ALL SOURCE INPUT
C END SOURCE
*
END CONTROL ! End of CONTROL keyword group
*
VOLUMES 5 ! total number of control volumes
* total MCO gas volume is 0.55 m3, 0.55/5=0.11 per each node
* No more than 5 columns (regions) at a time
*
VOLUME m3, SED_AREA m2, ELEVATION m, TEMP_GAS K, PRESSURE Pa
*
REGIONS      1      2      3      4      5
VOLUME      0.183      0.183      0.183      0.25      1.E9
SED_AREA     0.172      0.172      0.172      0.0      0.0
ELEVATION    2.65      1.33      700.15      700.5      700.15
TEMP_GAS     700.15      700.15      700.15      700.5      700.15
PRESSURE     1.0135      1.0135      1.0135      1.0135      1.0135
END REGIONS ! REGIONS is a comment
* If there are more than five regions, continue here
*
REGIONS      6      7
VOLUME      0.183      1.E9
SED_AREA     0.27      0.0
ELEVATION    0.0      0.0
TEMP_GAS     173.15      0.85
PRESSURE     1.0475      1.0475
END REGIONS ! REGIONS is a comment

```


Date: 12/31/98

THSFIX 42 2 50.0 50.0

END HEAT_SINKS ! HEAT_SINKS is a comment

JUNCTIONS 3 1 3 Junctions

1) MCO bottom to MCO middle, 3->2
2) MCO middle to MCO top, 2->1
3) MCO top to outlet volume, 1->5 (deactivated)

* Syntax: Junction Type: 1 = Normal, 2 = HEPA, 3 = Cover

* IRTYP Upstream Region

* IR2 Downstream Region

* AJN Bypass area for HEPA junction (m^2)

* AHP HEPA Filter Failure Pressure (Pa)

* HEPA Cover Area (m^2)

* MCOV Cover Weight (kg)

* 21JN Elevation wrt floor of IRI opening (m)

* 22JN Loss coefficient multiplies 0.5rho*v^2

* CJN Orientation: 1 = horizontal, 0 = vertical

* IORIZ Characteristic width, m

* XWJN Characteristic height, m

* XWJN Characteristic length, m

* XWJN Decontamination Factor

* N90 No. of 90 bends

* PATHS 1 2 3

1) IRTYP 1 1 1

2) IRTYP 2 1 1

3) IRTYP 3 1 1

4) IRTYP 4 1 1

5) IRTYP 5 1 1

6) IRTYP 6 1 1

7) IRTYP 7 1 1

8) IRTYP 8 1 1

9) IRTYP 9 1 1

10) IRTYP 10 1 1

11) IRTYP 11 1 1

12) IRTYP 12 1 1

13) IRTYP 13 1 1

14) IRTYP 14 1 1

15) IRTYP 15 1 1

16) IRTYP 16 1 1

17) IRTYP 17 1 1

18) IRTYP 18 1 1

19) IRTYP 19 1 1

20) IRTYP 20 1 1

21) IRTYP 21 1 1

22) IRTYP 22 1 1

23) IRTYP 23 1 1

24) IRTYP 24 1 1

25) IRTYP 25 1 1

26) IRTYP 26 1 1

27) IRTYP 27 1 1

28) IRTYP 28 1 1

29) IRTYP 29 1 1

30) IRTYP 30 1 1

31) IRTYP 31 1 1

32) IRTYP 32 1 1

33) IRTYP 33 1 1

34) IRTYP 34 1 1

35) IRTYP 35 1 1

A 76

500.0
CVI 0.0
XVI 0.0
XRO 0.0127
AHS 1.32
TIMT 700.00
TOINIT 700.00
INSLAB 1
IREGI 0.0
TIHS 4
IREGO 0.0
TIHS 3.95
EHSI 0.3
EHSO 0.3
END

CASK WALL MCO BOT MCO LID
42 43 44
0 8000.0 8000.0
RHO 7753.0 16.0
KHS 36.0 500.0
XHS 486.0 0.0
CVI 0.0 0.0
XVI 0.0 0.0
XRO 0.0 0.0
AHS 0.3192 0.045 0.23
TIMT 18.4 700.00 700.00
TOINIT 700.00 700.00 700.00
INSLAB 10 10 10
IREGI 4 3 3
IREGO 0.0 0.0 0.0
TIHS 0.0 0.0 0.0
EHSI 0.0 0.0 0.0
EHSO 3.950 0.3 0.3
TIMT 0.25 0.25 0.25
TOINIT 0.25 0.25 0.25
INSLAB 0.25 0.25 0.25
IREGI 0.25 0.25 0.25
IREGO 0.25 0.25 0.25
TIHS 0.25 0.25 0.25
EHSI 0.25 0.25 0.25
EHSO 0.25 0.25 0.25
END

USER CAN CONTROL HEAT SINK BOUNDARY TEMPERATURE
* SYNTAX:
* OFFSET TIMES
* EXTRAPOLATION TIMES
* TIMHS IHS ISD - TIME1, TIME2...
* THSFIX IHS ISD - TIME1, TIME2...
* IHS = HEAT SINK NO. 1 - 50, SIDE NO. (1 OR 2) FOR IHS
* CONTROL HEAT SINK BOUNDARY T
* OFFSET_TIMES TIMES EXTRAP
* TIMES 15 2 0.0 1.56
* TIMES 15 2 50.0 50.0
* TIMES 15 2 0.0 1.56
* TIMES 15 2 50.0 50.0
* TIMES 30 2 0.0 1.56
* TIMES 30 2 50.0 50.0
* TIMES 41 2 0.0 1.56
* TIMES 41 2 50.0 50.0
* TIMES 42 1 50.0 50.0
* THSFIX 42 1 50.0 50.0
* THSFIX 42 2 0.0 1.56
* THSFIX 42 2 0.0 1.56

A - 77

FBI/98-40, Rev. 1

END IHSELF for 1st fuel basket

* 2nd Fuel Basket

* heat sink pairs for second fuel basket

IHSFL 1 2 3 4 5 6 7 8 9 10 11 12 13 14

* define the heat sinks comprising the first fuel basket (must be in pairs, for inner and outer elements)

* IFINS 0 ! define the adjacent center insert heat sink,

* IFMCO 15 ! define the adjacent MCO wall heat sink

* IFLLID 0 ! define the lid or floor heat sink to which the fuel radiates to

* AFLEL 0.131 ! flow area in the basket

* fraction of geometric area exposed for oxidation

* - area available for oxidation/floor heat sink area

* 6.8 m² / (2x3.6 m²) = 0.10119

PROXEL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

FOX 10.0 0.0 ! multiplier for PROXEL

XFLXO 0.0 ! initial oxide (oxide+hydride) thickness

* (to be applied to exposed area)

* FHYDO 0.0 ! fraction of initial oxide which is hydride

* initial amount (kg) of water per geometric surface area (m²) of fuel

* 4 kg / (6.8 m²) = 0.588

FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

FWELIO 0.0 ! on the outer surface of the insert

FWELMO 0.0 ! on the inner surface of the MCO wall

FAMEL 0.1 ! wetted fraction of MCO wall

FAMELM 1.0 ! wetted fraction of MCO wall

MSLEL 45.0 ! mass of sludge particles (kg) in the fuel basket

* 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,

* outer surface of outer fuel elements,

* and the MCO wall. Therefore, the dimension of the square matrix is

* 1-number of fuel rods+1. If there is no insert, number of fuel rods+1.

FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000

0.316 0.027 0.316 0.158 0.018 0.009 0.000 0.000

0.176 0.316 0.000 0.167 0.158 0.009 0.009 0.000

0.018 0.316 0.334 0.167 0.316 0.316 0.167 0.022

0.000 0.018 0.158 0.000 0.018 0.158 0.208

0.000 0.009 0.000 0.158 0.018 0.000 0.048 0.558

0.000 0.000 0.018 0.167 0.176 0.343 0.460 0.106

0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106

* gap distance for micro-convection calculation

XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000

0.037 0.000 0.037 0.037 0.056 0.000 0.000 0.000

0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000

0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090

0.000 0.056 0.037 0.037 0.056 0.000 0.037 0.056

0.000 0.000 0.037 0.037 0.056 0.000 0.037 0.043

0.000 0.000 0.000 0.037 0.037 0.056 0.000 0.043

END IHSELF for 1st fuel basket

* 2nd Fuel Basket

* heat sink pairs for second fuel basket

IHSFL 16 17 18 19 20 21 22 23 24 25 26 27 28 29

* define the heat sinks comprising the first fuel basket (must be in pairs, for inner and outer elements)

* IFINS 0 ! define the adjacent center insert heat sink,

* IFMCO 30 ! define the adjacent MCO wall heat sink

* IFLLID 43 ! define the lid or floor heat sink to which the fuel radiates to

* AFLEL 0.131 ! flow area in the basket

* fraction of geometric area exposed for oxidation

* - area available for oxidation/floor heat sink area

* 6.8 m² / (2x3.6 m²) = 0.10119

PROXEL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

FOX 10.0 0.0 ! multiplier for PROXEL

XFLXO 0.0 ! initial oxide (oxide+hydride) thickness

* (to be applied to exposed area)

* FHYDO 0.0 ! fraction of initial oxide which is hydride

* initial amount (kg) of water per geometric surface area (m²) of fuel

* 4 kg / (6.8 m²) = 0.588

FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

FWELIO 0.0 ! on the outer surface of the insert

FWELMO 0.0 ! on the inner surface of the MCO wall

FAMEL 0.1 ! wetted fraction of MCO wall

FAMELM 1.0 ! wetted fraction of MCO wall

MSLEL 45.0 ! mass of sludge particles (kg) in the fuel basket

* 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,

* outer surface of outer fuel elements,

* and the MCO wall. Therefore, the dimension of the square matrix is

* 1-number of fuel rods+1. If there is no insert, number of fuel rods+1.

FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000

0.316 0.027 0.316 0.158 0.018 0.009 0.000 0.000

0.176 0.316 0.000 0.167 0.158 0.009 0.009 0.000

0.018 0.316 0.334 0.167 0.316 0.316 0.167 0.022

0.000 0.018 0.158 0.000 0.018 0.158 0.208

0.000 0.009 0.000 0.158 0.018 0.000 0.048 0.558

0.000 0.000 0.018 0.167 0.176 0.343 0.460 0.106

0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106

* gap distance for micro-convection calculation

XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000

0.037 0.000 0.037 0.037 0.056 0.000 0.000 0.000

0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000

0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090

0.000 0.056 0.037 0.037 0.056 0.000 0.037 0.056

0.000 0.000 0.037 0.037 0.056 0.000 0.037 0.043

0.000 0.000 0.000 0.037 0.037 0.056 0.000 0.043

Date: 12/31/98

A 79

FAI/98-40, Rev. 1

END MCO

A.14B Nitriding Validation # 2

```

0.000 0.000 0.000 0.000 0.090 0.056 0.043 0.000
END IHSLF for 2nd fuel basket
END FUEL_BSKT
* SCRAP_BSKT 1 ! Total number of scrap baskets
* IHSCC 31 ! ring 1, theta
32 33 ! ring 2, theta
34 35 ! ring 3 & 4, radial
37 36 ! ring 6 & 5, radial
38 39 ! ring 11 & 12, radial
* ISCONS 0 ! define the adjacent center insert heat sink,
! define the adjacent center insert heat sink
! define the adjacent center insert heat sink
! define the adjacent center insert heat sink
! define the lid or floor heat sink to which the
scrap
! radiate to
* porosity of the scrap for each heat sink in the order read in
(31, 32, 33, 34, ..)
* PFOROS 0.45 0.45 0.45 0.45 0.6 0.6 0.6 0.6
* characteristic size for each scrap heat sink in the order read in (m)
XHSCCR 0.00635 0.00635 0.00635 0.00635 0.00635
XHSCCR 0.0254 0.0254 0.0254 0.0254
XHSCBK 0.2860 ! radius of scrap basket (m)
XHSCBK 0.691 ! height of scrap basket (m)
* exposed surface area available for oxidation
* per unit volume of scrap (l/m) for the order read in
* each scrap basket heat sink in the order read in
* Example: bounding oxidation area: 6/0.17491 = 34.30 m^2
* 6 m^2 fine oxidation area: 10/0.01756 = 569.48 m^2/m^3
* 5.4 m^2 coarse oxidation area: 5.4/0.15734 = 34.32 m^2/m^3
*
* AVONSC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
* FOMSC 10.0 ! multiplier for AVONSC
* XSCOXO 0.0 ! initial oxide thickness on the exposed surface (m)
*
* PSCHYD 0.0 ! fraction of oxide which is hydride
* 1.5 kg of water to be for scrap basket; 1.5/0.17491 = 8.576 kg/m^3
* AVHSCO 8.576 ! initial amount (kg) of water per unit bulk volume
* FMSCTO 0.0 ! (m^3) of scrap
* ! on the outer surface of the insert
* ! (per unit area, m^2)
* FMSCMO 0.0 ! (per unit area, m^2) on the inner surface of the MCO wall
* ! (per unit area, m^2) on the surface area
* FAWSC 0.1 ! wetted fraction of MCO wall
* FAWSCM 1.0 ! gap, distance between the insert and scrap basket
* XSCXTN 0.01 ! gap, distance between the insert and MCO wall
* XSCWCO 0.00635 ! gap distance between scrap basket and MCO wall
* XSCWCO 55.0 ! mass of sludge particles (kg) in the scrap basket
* END IHSCF for 1st scrap basket
* END SCRAP_BSKT
* END MCO

```

```

* TITLE ! Keyword; next line is title, title can be any length
NITRIDE - NITRIDING VALIDATING AT 800 C
END TITLE ! Anything after END is a comment
*
* TIMING ! Keyword
TSTART 0. ! START TIME, >0 FOR RESTART RUN
! RESTART FILE IS READ FROM HANSF.NER
! END TIME (Seconds)
! MIN TIMESTEP (Seconds)
! MAX TIMESTEP (Seconds)
! PRINT INTERVAL (Seconds)
! MIN PLUG INTERVAL (Seconds)
! MAX PLUG INTERVAL (Seconds)
! RESTART INTERVAL WITHOUT PLOT (Seconds)
! RESTART INTERVAL (Seconds)
! FRACTIONAL CHANGE IN T AND P
! FRACTIONAL CHANGE IN AEROSOL MASS
! FRACTIONAL CHANGE FOR PLOTTING
END TIMING ! TIMING is a comment.

```

```

* PLOT ! Keyword for plotting section
* Plotting syntax:
* PRESSURE n rlist - Pressure, Pa
* GAS-T n rlist - Gas Temperature, K
* HS-T n rlist - Heat Sink Temperature - Inner Surface, K
* HS-T n rlist - Heat Sink Temperature - Outer Surface, K
* HS-TA n rlist - Heat Sink Temperature - Average, K
* AEROSOL n rlist - Aerosol Mass (Total), kg
* GAS-W n rlist - Mass Flowrate, kg/s
* GAS-WX n rlist - CounterCurrent Mass Flowrate, kg/s
* GAS-X n rlist - Gas Relative Humidity
* GAS-RH n rlist - Gas Relative Humidity
* GAS-MASS n rlist - Gas Mass (Species), kg
* GAS-MASS n rlist - Gas Mass (Species), kg
* GAS-MASS n rlist - Total Mass (Species), kg

```

```

CONTROL ! Major keyword group

```

```

* NITRIDE MODEL TEST NITRID.DAT

```

```

* T=800 C, NO DECAY HEAT

```

```

* UNLESS OTHERWISE NOTED, MMS UNITS

```

```

* - 1 TIER OF SCRAP BASKET

```

```

* - 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)

```

```

* LIQ-MASS - GASNAME n list - Deposited Mass (Species), kg
* Pressure, Gas Temperature, and total aerosol mass require a region
* list
* Heat Sink Temperatures need a heat sink number list
* Flowrates need a junction number list
* Gas concentration, relative humidity, individual species gas mass,
  individual species aerosol mass, total (gas+aerosol) individual
  species mass, and individual species deposited liquid mass require
  a region and gas name
  PRESSURE 1 1 2 3 4 5 ! Pressure in MCO
  GAS-T 11 31 32 33 34 35 36 37 38 39 40 ! Temp in region
  HS-TI 13 41 42 43 44 45 ! Cask, bottom, and lid
  HS-TA 15 12 13 14 15
  HS-TA 16 17 18 19 20 21 22 23 24 25 ! Bot. fuel
  HS-TA 10 16 17 18 19 20 21 22 23 24 25 ! Bot. fuel
  HS-TA 5 26 27 28 29 30
  GAS-X NITROGEN 3 1 2 3 ! N2 concentration in MCO
  GAS-X OXYGEN 3 1 2 3 ! O2 concentration in MCO
  GAS-X STEAM 3 1 2 3 ! H2O concentration in MCO
  GAS-X HYDROGEN 3 1 2 3 ! H2 concentration in MCO
  GAS-X HELIUM 3 1 2 3 ! He concentration in MCO
  GAS-XK 3 1 2 3 ! Uni-directional mass flowrate
  GAS-XK 3 1 2 3 ! Counter-current mass flowrate
  GAS-MASS HYDROGEN 1 5 ! Mass of hydrogen in region 5
  GAS-MASS STEAM 1 5 ! Mass of steam in region 5
  END PLOT ! PLOT is a comment
  
```

```

ACTIVE MODELS ! Keyword; MODELS is a comment; 1 = on, 0 = off
  LUNAR 1 ! Lunar flow model
  THIN 1 ! Counter-current flow model
  THIN 1 ! Heat sinks
  THIN 1 ! Condensation
  TASED 0 ! Aerosol Sedimentation
  TALEAK 0 ! Aerosol Leakage
  IFOG 0 ! Fog formation
  ISRC 0 ! User-defined sources
  IMCO 0 ! MCO activity runs
  ISM 0 ! SMO activity runs
  END ACTIVE MODELS ! ACTIVE MODELS is a comment
  
```

```

SOURCE GROUP! GROUPS REPEATED FOR INPUT # OF REGIONS
END OF GROUP! GROUPS REPEATED BY 'REGION' OR 'END' KEYWORDS
  FLOWRATES, FLOWRATES, POWER
  SYNTAX EXAMPLE:
    SOURCES:2 1 -- KEYWORD AND # SOURCE GROUPS
    REGION 1 GASES 2 1 -- REGION #, # GASES
    STEAM HYDROGEN 1 -- GAS NAMES MUST BE ON NEXT LINE
    0 300 1.E-3 1.E-3 0.E0
    10 300 1.E-3 1.E-3 0.E0
  
```

```

--- ENDS A REGION SOURCE
--- FOR AEROSOL, SPECIFY -IVE REGION

END REGION
REGION -1 GASES 1
  NAL 300.0 4.44E-1 0.E0
  10. 300.0 4.44E-1 0.E0
  900. 300.0 4.44E-1 0.E0
  901. 300.0 0.E0 0.E0
  1.E5 300.0 0.E0 0.E0
  END REGION
END SOURCE
!--- ENDS A REGION SOURCE
!--- ENDS ALL SOURCE INPUT

END CONTROL ! End of CONTROL keyword group

VOLUMES 5 ! total number of control volumes
! total MCO gas volume is 0.55 m^3, 0.55/3=0.183 per each node
! With more than 5 columns (regions) at a time
! VOLUME m^3, SED_AREA m^2, ELEVATION m, TEMP GAS K, PRESSURE Pa
  REGIONS 1 2 3 4 5
  MCO top MCO middle MCO bottom gap environment
  VOLUME 0.183 0.183 0.183 0.25 1.89
  SED_AREA 0.172 0.172 0.172 0.0 0.0
  ELEVATION 373.15 299.85
  PRESSURE 1.047E5 1.047E5
  END REGIONS ! REGIONS is a comment
  ! Gas composition of each region; specify mole fraction of each gas
  ! No more than five columns at a time
  GASES 1 2 3 4 5
  REGION 0.1 0.1 0.1 0.1 0.0
  STEAM 0.0 0.0 0.0 0.0 0.010
  OXYGEN 0.0 0.0 0.0 0.0 0.205
  NITROGEN 0.9 0.9 0.9 0.9 0.785
  WATER 0.0 0.0 0.0 1.0 0.0
  END GASES ! GASES is a comment
  ! If there are more than five regions, continue here.
  
```


A - 84

IROUIM - Pump outlet region
 IROUIM - Note to which the condensed steam is dumped for back-keeping
 IROUIM - If non-zero, overrides TGFED with the designated region
 IROUIM - Temperature. Used to specified time-varying feed
 temperature
 WVPUMP - Pump volumetric flowrate (m³/s)
 WVPUMP - Feed volumetric flowrate (m³/s)
 TGFED - Feed temperature (K)
 TCONPM - Condenser cooling coil temperature (K)
 35 FT³/MIN + 1 MIN/60 SEC + 0.02832 M³/1 FT³ = 0.01652 M³/SEC
 PUMP IROUIM IROUIM IROUIM IROUIM IROUIM IROUIM IROUIM IROUIM IROUIM IROUIM
 PUMP 1 5 0 0 1.652E-2 0.0 0.0 0.0
 Radiolysis parameters
 FRAD 1.0 ! multiplier for radiolysis
 ALPHA 0.197 ! alpha fractional heat load
 BETA 0.486 ! beta fractional heat load
 GAMMA 0.317 ! gamma fractional rate in MCO free water per gram
 QPHOTO 2.4E-6 ! heat WU of fuel loading
 ! GENERAL is a comment
 END GENERAL
 SOLAR_RAD
 ! pointers to heat sinks representing the cask wall and the top
 ! solar radiation impinges on these
 IHCA5K 42
 IHTOP 44
 ! look-up table for solar radiation throughout a day (sec vs. W/m²)
 OFFSET_TMDAY 21600. ! offset by six hours
 EXTRAPOLATION_TMDAY PERIOD 0.10000 0.14000 0.18000 0.21600.0
 0.0 3600.0 32400.0 36000.0 39600.0 43200.0 46800.0
 TMDAY 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
 75600.0 79200.0 82800.0 86400.0
 RADSON 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 END SOLAR_RAD
 FUEL_BSKT 2 ! Total number of fuel baskets
 ! 1st Fuel Basket
 IHSTFL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
 ! define the heat sinks comprising the first fuel basket (must be
 ! in pairs, for inner and outer elements)
 !FLINS 0 ! define the adjacent center insert heat sink,
 0 for no insert
 IFMCO 15 ! define the adjacent MCO wall heat sink
 IFILLD 0 ! define the lid of floor heat sink to which the fuel
 ! radiate to

ATLEFL 0.131 ! flow area in the basket
 * fraction of geometric area exposed for oxidation
 * area available for oxidation/total heat sink area
 * 6.8 m² / (2*33.6 m²) = 0.10119
 FAXCEL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
 FOX 10.0 0.0 ! multiplier for FAOXFL
 FOXOX 0.0 ! initial oxide (oxide+hydride) thickness
 ! (to be applied to exposed area)
 FXHYD0 0.0 ! fraction of initial oxide which is hydride
 * initial amount (kg) of water per geometric surface area (m²) of fuel
 * 24 kg / (2*33.6 m²) = 0.3571
 FWEL0 8.6/2/16.8 = 0.256 kg/m² (per side)
 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
 FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
 FWEL0 0.0 ! on the outer surface of the insert
 FWEL0 0.0 ! on the inner surface of the MCO wall
 FWEL0 0.0 ! wetted fraction of fuel surface
 FWEL0 0.0 ! wetted fraction of MCO wall
 FWEL0 1.0 ! mass of sludge particles (kg) in the fuel basket
 FWEL0 45.0 ! 22.5 kg per fuel basket x 2 baskets = 45 kg
 * view factor matrix between the insert,
 * outer surface of outer fuel element,
 * and the MCO wall. The first row is the dimension of the square matrix is
 * i number of fuel rods. If there is no insert, number of fuel
 * rods=1.
 FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000 0.000
 0.316 0.027 0.316 0.158 0.018 0.000 0.000 0.000 0.000
 0.176 0.316 0.000 0.167 0.316 0.000 0.009 0.000
 0.018 0.316 0.334 0.158 0.000 0.316 0.167 0.022
 0.000 0.018 0.000 0.158 0.000 0.018 0.158 0.107
 0.000 0.000 0.000 0.158 0.018 0.000 0.158 0.208
 0.000 0.000 0.018 0.167 0.316 0.316 0.048 0.558
 0.000 0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
 * gap distance for micro-convection calculation
 XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
 0.037 0.000 0.037 0.056 0.056 0.056 0.056 0.000
 0.037 0.037 0.000 0.000 0.037 0.000 0.037 0.000
 0.056 0.036 0.037 0.037 0.000 0.056 0.037 0.000
 0.000 0.056 0.000 0.037 0.056 0.000 0.037 0.056
 0.000 0.000 0.037 0.037 0.037 0.037 0.000 0.043
 0.000 0.000 0.000 0.000 0.090 0.090 0.056 0.000
 END IHSTFL for 1st fuel basket
 * 2nd Fuel Basket
 * heat sink pairs for second fuel basket
 IHSTFL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
 !FLINS 0 ! define the adjacent center insert heat sink,
 ! 0 for no insert

Date: 12/31/98

A - 86

```

IFMLCO 30 ! define the adjacent MCO wall heat sink
IFMLID 43 ! define the lid or floor heat sink to which the fuel
          ! radiates to
AFIPL 0.131 ! flow area in the basket,
* fraction of geometric area exposed for oxidation
* 6.8 m2 / (243.6 m2) = 0.10119
FACFEL 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
FOX 10.0 0.0 ! multiplier for FACFEL
FXFLOX 0.0 ! initial oxide (oxide-hydride) thickness
FXHYD 0.0 ! (to be applied to exposed surface)
* initial amount (kg) of water per geometric surface area (m2) of fuel
*
FWFLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
FWFLO 0.0 ! on the outer surface of the insert
FWFLO 0.4545 ! on the inner surface of the MCO wall
FWFLO 0.4545 ! on the inner surface of fuel element
FWFLO 0.1 ! wetted fraction of MCO wall
FWFLO 0.1 ! wetted fraction of fuel element
FWFLO 45.0 ! mass of sludge particles (kg) in the fuel basket
FWFLO 45.0 ! 22.5 kg per fuel basket x 2 basket = 45 kg
*
* view factor matrix between the insert,
* outer surface of outer fuel element,
* and the MCO wall. If there is no insert, the dimension of the square matrix is
* the number of fuel rods. If there is no insert, number of fuel
* rods = 1.
FVUEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
0.316 0.027 0.316 0.158 0.018 0.009 0.009 0.000
0.176 0.316 0.000 0.167 0.316 0.316 0.167 0.022
0.018 0.316 0.158 0.018 0.000 0.018 0.158 0.107
0.000 0.009 0.000 0.158 0.018 0.000 0.158 0.208
0.000 0.000 0.018 0.167 0.316 0.316 0.048 0.558
0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
*
* gap distance for micro-convection calculation
*
XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.000 0.030 0.037 0.056 0.056 0.000 0.000
0.037 0.037 0.037 0.037 0.000 0.037 0.000 0.000
0.056 0.037 0.037 0.000 0.037 0.000 0.037 0.037
0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.037
0.000 0.056 0.000 0.037 0.056 0.000 0.037 0.056
0.000 0.000 0.037 0.037 0.037 0.037 0.037 0.043
0.000 0.000 0.000 0.037 0.037 0.037 0.037 0.000
END IHSEL for 2nd fuel basket
END FUEL_BSKT
*
* SCRAP_BSKT 1 ! Total number of scrap baskets
*
IHSC 31 ! ring 1, theta
32 33 ! ring 2, theta
34 35 ! ring 3 & 4, radial
37 36 ! ring 6 & 5, radial
38 39 ! ring 11 & 12, radial
*
* IHSCINS 0 ! define the adjacent center insert heat sink,
* ! for no insert
* ! define the adjacent MCO wall heat sink
* ! define the lid or floor heat sink to which the
* ! radiate to
*
* porosity of the scrap for each heat sink in the order read in
* (31, 32, 33, 34, ..)
PFOROS 0.45 0.45 0.45 0.45 0.45 0.45 0.6 0.6 0.6
* characteristic size for each scrap heat sink in the order read in (m)
* 0.00235 0.00235 0.00235 0.00235 0.00235 0.00635
XDCRCP 0.00235 0.00235 0.00235 0.00235 0.00235
YRSCBK 0.2860 ! radius of scrap basket (m)
XHSCBK 0.691 ! height of scrap basket (m)
*
* exposed surface area available for oxidation
* per unit volume of scrap (1/m) for
* each scrap basket heat sink in the order read in
*
* Example: bounding oxidation area: 6/0.17491 = 34.30 m2
* 10 m2 fine oxidation area: 10/0.01756 = 569.48 m2/m3
* 10 m2 fine oxidation area: 10/0.01756 = 569.48 m2/m3
* 5.4 m2 coarse oxidation area: 5.4/0.15734 = 34.32 m2/m3
*
AVOYSC 34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30
FOYSC 10.0 ! multiplier for AVOYSC
XSCOX 0.0 ! fraction of oxide thickness on the exposed surface (m)
XSCOX 0.0 ! fraction of oxide which is hydride
* 15.5 m2 of water total for scrap basket; 1.5/0.17491 = 8.576 kg/m3
WVNSCO 8.576 ! initial amount (kg) of water per unit bulk volume
(m3) of scrap
FWSCIO 0.0 ! on the outer surface of the insert
FWSCIO 0.0 ! on the inner surface of the MCO wall
FWSCIO 0.0 ! on the inner surface of fuel element
FMSC 0.1 ! (per unit surface area)
FMSC 1.0 ! wetted fraction of MCO wall
XSCINS 0.01 ! gap distance between the insert and scrap basket
1/4" gap for scrap basket and MCO wall
XSCWCO 0.00635 ! gap distance between scrap basket and MCO wall
MSLSC 55.0 ! mass of sludge particles (kg) in the scrap basket
END THESC for 1st scrap basket
END SCRAP_BSKT
*
* END MCO

```

A.14C Nitriding Validation # 3

 * NITRIDE MODEL TEST - NITRID3.DAT
 * T=160 C, NO DECAY HEAT
 * UNLESS OTHERWISE NOTED, MKS UNITS
 *

FAI/98-40, Rev. 1

A - 87

FAY/98-40, Rev. 1

* No more than five columns at a time, so continue with 6 & 7

```

* AEROSOLS 6 7
* STEAM 0.0 0.0
* END AEROSOLS ! AEROSOLS is a comment

* OPTIONAL TEMPERATURE AND PRESSURE CONTROL
* CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
* IMPOSE TEMPERATURE LOOK-UP TABLE
* SYNTAX:
* OFFSET TIMEPG
* MCO REGION TIMEPG
* TIMEPG IREG TIME1, TIME2...TIMELAST
* TGFIX IREG TIME1, TIME2...TEMPLAST
* LINEAR INTERPOLATION BETWEEN VALUES
* SIMILAR SYNTAX FOR PRESSURE:
* OFFSET TIMEPG
* EXTRAPOLATION TIMEPG
* TIMEPG IREG TIME1, TIME2...
* TGFIX IREG PRES1, PRES2...PRESSURES ARE IN PA!!!
* OFFSET_TIMEPG= OFFSET TIME; ENTER LOOKUP TABLE WITH
* TIME-OFFSET_TIMEPG
* EXTRAPOLATION_TIMEPG= LAST TO USE LAST VALUE IN THE TABLE.
* = EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
* = PERIOD TO WRAP AROUND.

* OFFSET_TIMEPG 500
* EXTRAPOLATION_TIMEPG LAST
* TIMEPG 1 0.0 100. 200.
* TGFIX 1 293.15 373.15 473.15

* CONTROL MCO BOUNDARY P, 30.
* OFFSET_TIMEPG
* EXTRAPOLATION_TIMEPG
* TIMEPG 1 0.0 100. 200.
* TGFIX 1 1.25 1.25 1.45
* END VOLUMES ! VOLUMES is a comment

* Major keyword-----
* HEAT_SINKS 44 ! Total number of heat sinks
* decay power based on 835 W per MCO.
* No more than 5 columns at a time,
* Repeat the following structure,
* SINKS
*
*
*
*
* END

* Syntax:
* TGSOM 1 for plane, 0 or 2 for cylinder
* RHO Density (kg/m3)
* K Conductivity (W/m/K)
* CPHS Specific Heat (J/kg/K)
* QV Volumetric Heat Generation (W/m3)

```

```

* END CONTROL ! End of CONTROL keyword group
*
*
*-----
* VOLUMES 5 ! total number of control volumes
* total MCO gas volume is 0.55 m3, 0.3572=0.183 per each node
* No more than 5 columns (regions) at a time
* Units:
* VOLUME m3, SED_AREA m2, ELEVATION m, TEMP_GAS K, PRESSURE Pa
*
* REGIONS
* MCO top MCO middle MCO bottom gap environment
* 1 2 3 4 5
* VOLUME 0.183 0.183 0.183 0.25 1.89
* SED_AREA 0.172 0.172 0.172 0.0 0.0
* ELEVATION 1.33 760.00 760.00 760.00
* TEMP_GAS 323.15 299.85
* PRESSURE 1.01325 1.01325 1.01325 1.01325
* END REGIONS ! REGIONS is a comment
* If there are more than five regions, continue here
*
* REGIONS 7
* VOLUME 0.183 1.89
* SED_AREA 0.27 0.0
* ELEVATION 0.0 0.0
* TEMP_GAS 323.15 299.85
* PRESSURE 1.01325 1.04755
* END REGIONS ! REGIONS is a comment
* Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
*
* GASES 2 3 4 5
* HELIUM 0.1 0.1 0.0 0.0
* STEAM 0.0 0.0 0.0 0.010
* OXYGEN 0.0 0.0 0.0 0.205
* NITROGEN 0.0 0.9 0.9 0.785
* END GASES ! GASES is a comment
*
* If there are more than five regions, continue here.
*
* GASES 6 7
* HELIUM 0.89 0.0
* STEAM 0.11 0.0158
* OXYGEN 0.0 0.2067
* NITROGEN 0.0 0.7775
* WATER 0.0 0.0
* END GASES ! GASES is a comment
* Aerosol concentration of each region (kg/m3)
* No more than five columns at a time
*
* AEROSOLS 1 2 3 4 5
* STEAM 0.0001 0.0 0.0 0.0
* END AEROSOLS ! AEROSOLS is a comment

```

Inner Radius (m); for plane wall, thickness = XRO-XRI														
* XRI	Outer Radius (m); for plane wall, thickness = XRO-XRI													
* XRO	One-sided heat sink area (m ²)													
* AHS	Initial inside surface temperature (C)													
* TOINIT	Initial outside surface temperature (C)													
* TOINSLAB	Number of slabs; 3 is minimum													
* IREGI	Region index for inner surface or 0 (insulated)													
* TIHS	Region index for outer surface when IREGI = -1 (C)													
* IREGO	Region index for outer surface or 0 (insulated)													
* XHS	or -1 for constant temperature													
* AHS	Region surface temperature when IREGO = -1 (C)													
* TOINIT	Characteristic length for natural convection (m)													
* XHS	Emissivity of inner surface													
* EHSI	Emissivity of outer surface													
* EHSO	Emissivity of outer surface													
* Fuel Basket #1 heat sinks 1 through 15														
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* SINKS														

FANFL 0.1 ! wetted fraction of fuel surface
 FANFLM 1.0 ! wetted fraction of MCO wall
 MSFL 45.0 ! mass of sludge particles (kg) in the fuel basket
 MSFL 45.0 ! 22.5 kg per fuel basket x 2 basket = 45 kg

* view factor matrix between the insert,
 * and the MCO wall. Therefore, the dimension of the square matrix is
 * nnumber of fuel rods+1. If there is no insert, number of fuel
 * rods+1.

FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
 0.316 0.027 0.316 0.159 0.028 0.000 0.000 0.000
 0.176 0.316 0.392 0.167 0.316 0.316 0.167 0.022
 0.018 0.018 0.158 0.158 0.000 0.018 0.158 0.107
 0.000 0.009 0.000 0.158 0.018 0.000 0.158 0.208
 0.000 0.000 0.018 0.167 0.316 0.048 0.158
 0.000 0.000 0.018 0.176 0.343 0.460 0.156

* gap distance for micro-convection calculation

XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
 0.037 0.000 0.037 0.037 0.056 0.056 0.000 0.000
 0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000
 0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090
 0.000 0.056 0.037 0.037 0.000 0.06 0.037 0.056
 0.000 0.056 0.000 0.037 0.037 0.000 0.037 0.043
 0.000 0.000 0.000 0.037 0.037 0.037 0.000 0.043

END IHSELF for 1st fuel basket

* 2nd Fuel Basket

* heat sink pairs for second fuel basket

IHSELF 16 17 18 19 20 21 22 23 24 25 26 27 28 29
 IFLINS 0 ! define the adjacent center insert heat sink,
 ! 0 for no insert
 IFLMCO 30 ! define the adjacent MCO wall heat sink
 IFLMID 43 ! define the lid or floor heat sink to which the fuel
 ! radiate to

AFELF 0.131 ! flow area in the basket,

* fraction of geometric area exposed for oxidation
 * 6.8 m² / 0.131 m² = 0.10119
 FANFLM 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119
 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119 0.10119

FOX 10.0 ! multiplier for FOXFL

XFLOXO 0.0 ! initial oxide (oxide+hydride) thickness

* (to be applied to exposed area)

FHYDRO 0.0 ! fraction of initial oxide which is hydride

* Initial amount (kg) of water per geometric surface area (m²) of fuel

FWELO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571

FWELO 0.0 ! on the outer surface of the insert

* 1 kg / 2.2 m² = 0.4545

FWELO 0.4545 ! on the inner surface of the MCO wall

* view factor matrix between the insert,
 * outer surfaces of fuel rods. Therefore, the dimension of the square matrix is
 * nnumber of fuel rods+1. If there is no insert, number of fuel
 * rods+1.

FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
 0.316 0.027 0.316 0.159 0.028 0.000 0.000 0.000
 0.176 0.316 0.392 0.167 0.316 0.316 0.167 0.022
 0.018 0.018 0.158 0.158 0.000 0.018 0.158 0.107
 0.000 0.009 0.000 0.158 0.018 0.000 0.158 0.208
 0.000 0.000 0.018 0.167 0.316 0.048 0.158
 0.000 0.000 0.018 0.176 0.343 0.460 0.156

* gap distance for micro-convection calculation

XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
 0.037 0.000 0.037 0.037 0.056 0.056 0.000 0.000
 0.037 0.037 0.000 0.037 0.037 0.000 0.037 0.000
 0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090
 0.000 0.056 0.037 0.037 0.000 0.056 0.000 0.037 0.090
 0.000 0.056 0.000 0.037 0.037 0.056 0.000 0.037 0.090
 0.000 0.000 0.037 0.037 0.037 0.056 0.037 0.056
 0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.043
 0.000 0.000 0.000 0.037 0.037 0.037 0.037 0.043

END IHSELF for 2nd fuel basket

END FUEL_BSKT

* SCRAP_BSKT 1 ! Total number of scrap baskets

IHSCN 31 ! ring 1, theta
 32 33 ! ring 2, theta
 34 35 ! ring 3 & 4, radial
 37 38 ! ring 8 & 9, radial
 38 39 ! ring 11 & 12, radial

* ISCINS 0 ! define the adjacent center insert heat sink,
 ! 0 for no insert

ISCIN 40 ! define copper fin heat sink

ISCMCO 41 ! define the adjacent MCO wall heat sink

ISCLID 44 ! define the lid or floor heat sink to which the

scrap ! radiate to

* porosity of the scrap for each heat sink in the order read in

* 32 33 34 0.45 0.45 0.45 0.45 0.6 0.6 0.6 0.6

* PROPS 0.45 0.45 0.45 0.45 0.635 0.00635 0.00635 0.00635

* characteristic size for each scrap heat sink in the order read in (m)

* XDCSRP 0.00635 0.00635 0.00635 0.00635 0.0254

* XSCBCK 0.2860 ! radius of scrap basket (m)

* XHSCBCK 0.691 ! height of scrap basket (m)

* exposed surface area available for oxidation

* per unit volume of scrap (1/m) for


```

- LOOK-UP TABLE CONTROL IMPLEMENTED
- WATERFILL IS IN THE MCO/CLKS GAP
- WATERFILL IS IN THE MCO/CLKS GAP
- WATERFILL HEAT TRANSFER FROM FUEL/SCRAP TO LID/FLOOR.
*****
CONTROL      I Major keyword group
*****
*
* TITLE      I Keyword; next line is title, title can be any length
* CVOZA      - HE RECUR AFTER VACUUM CYCLES, 0.0 M2
*
* END TITLE  I Anything after END is a Comment
*****
*
* TIMING      I Keyword
*
* TSTART      28009.
* TSTOP       0.0
*
* TLAST       200000.
* DVMIN       0.01
* DVMAX       2.0
* DPMIN       2000.
* DPMAX       200.
* PLTMIN      1000.
* PLTMAX      20000.
* DTST        0.005
* FTCH        0.05
* FACH        0.0
*
* FRACTIONAL CHANGE IN T AND P
* FRACTIONAL CHANGE IN ARGOL MASS
* FRACTIONAL CHANGE FOR PLOTTING
* FRACTIONAL CHANGE FOR PLOTTING.
*****

```

```
prom      ! keyword for plotting section
```

Plotting syntax:

- *** PRESSURE n list - Pressure, Pa
- *** HS-T n list - Gas Temperature, K
- *** HS-TT n list - Heat Sink Temperature - Inner Surface, K
- *** HS-TO n list - Heat Sink Temperature - Outer Surface, K
- *** HS-TA n list - Heat Sink Temperature - Average, K
- *** AEROSOL n list - Aerosol Mass (Total), kg
- *** GAS-M n list - Mass Flowrate, kg/s
- *** GAS-MX n list - CounterCurrent Mass Flowrate, kg/s
- *** GAS-N GASNAME n list - Gas Molar Fraction
- *** GAS-NR GASNAME n list - Gas Mass Fraction
- *** GAS-NR GASNAME n list - Gas Mass (Species), kg
- *** GAS-HS GASNAME n list - Gas Mass (Species), kg
- *** AER-HS GASNAME n list - Aerosol Mass (Species), kg
- *** MASS GASNAME n list - Total Mass (Species), kg
- *** LCQ-MASS - GASNAME n list - Deposited Mass (Species), kg
- *** Pressure, Gas Temperature, and total aerosol mass require a region
** list
- *** Heat Sink Temperatures need a heat sink number list
- *** Flowrates need a junction number list
- *** Gas concentration, relative humidity, individual species gas mass,
total aerosol mass, total (gas+aerosol) individual

Date: 12/31/98

* each scrap basket	heat sink in the order read in				
* 6 m ²	bunding oxidation area; 6/0.17491 = 34.30 m ²				
* 10 m ²	bunding oxidation area; 10/0.0756 = 569.48 m ² /m ³				
* 5.4 m ²	coarse oxidation area; 5.4/0.15734 = 34.32 m ² /m ³				
AVNSXC	34.30 34.30 34.30 34.30 34.30 34.30 34.30 34.30				
FOXSC	10.0 ! multiplier for AVNSXC				
XSCX00	0.0 ! initial oxide thickness on the exposed surface (m)				
FSCVHD	0.0 ! fraction of oxide which is hydride				
W	1.5 kg of water				
HWNSC0	8.576 ! initial amount (kg) of water per unit bulk volume				
	(m ³) of scrap				
FNSC10	0.0 ! on the outer surface of the insert				
	(per unit area, m ²)				
FNSC10	0.0 ! on the inner surface of the MCO wall				
	(per unit area, m ²)				
FANSC	0.1 ! wetted fraction of surface area				
FANSCM	1.0 ! wetted fraction of MCO wall				
XSCM01	0.0 ! gap distance between scrap basket and mco wall				
XSCM01	0.0 ! gap distance between scrap basket and mco wall				
XSCMCO	0.00435 ! gap distance between scrap basket and mco wall				
XSCMCO	55 ! gap distance between scrap basket and mco wall				
END INSCSC	for lat scrap basket				
END INSCSC	for lat scrap basket				
END SCRAP_BSXT					
* END MCO					

A.15 Pump Model Validation

- CV2DA - HE RECIRC AFTER VACUUM CYCLE, 6.0 M²
- UNLESS OTHERWISE NOTED, MKS UNITS
- 1 TIER OF SCRAP BASKET
- 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)
- IMPROVED VERSION PER
- VACUUM FLOW RATE IS 35 CFM INSTEAD OF 40 CFM
- SPEC. HEAT OVER TIME IS 8 HRS, SO GENERATE THE RESTANT FILE EVERY 2
- RUN TO TWO DAYS USING 0.2 SEC TIME STEP
- AMBIENT TEMPERATURE (CASK EXTERIOR) IS 80 F (26.7 C) INSTEAD OF 86 F (30 C)
- NEW HYDRATE MODEL IS USED
- REACTION OF NITROGEN WITH URANIUM IS ADDED
- CASK/PACK GAS AREA 1 INCH (0.0155 M) INSTEAD OF 1 INCH (0.0254 M)
- CASK/PACK GAS AREA PER FUEL BASKET IS 1.7 M²
- BOTH SIDES OF THE CASK AND OUTER SURFACE OF MCC WALL TEMPERATURES ARE FIXED USING NEW 'IMPOSED HEAT SINK SURFACE TEMPERATURE' FACILITY (DO AWAY WITH ARTIFICIALLY INCREASED EMISSIV) FOR WATER FILLED ANNULUS
- THE CASK HAS INNER DIAMETER OF 25.19" AND OUTER DIAMETER OF 39.81" (0.635 M AND 1.0157 M) THICK

A - 95

FAI/98-40, Rev. 1

SINKS					CASK WALL					MCO BOT					MCO LID				
5					42					43					44				
INSLAB	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
IREGI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
THS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TOHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
XLHS	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6
INSLAB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IREGI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
THS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TOHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
XLHS	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6
INSLAB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IREGI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
THS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TOHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
XLHS	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6
INSLAB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IREGI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
THS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TOHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
XLHS	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6
INSLAB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IREGI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
THS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TOHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
XLHS	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6
INSLAB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IREGI	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
THS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IREGO	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TOHS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
XLHS	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6	RS-6

END HEAT SINKS ! HEAT SINKS is a comment

JUNCTIONS 3 ! 3 Junctions

* 1) MCO Bottom to MCO Middle, 3->2

* 2) MCO Middle to MCO Top, 2->1

* 3) MCO Top to Outlet volume, 1->5 (deactivated)

* Syntax!

* Junction Type: 1 = Normal, 2 = HEPA, 3 = Cover

* IR1 Upstream Region

* IR2 Downstream Region

* A/JN Area (m^2)

* ABYP Bypass area for HEPA junction (m^2)

Date: 12/31/98

A - 100

FAI/98-40, Rev. 1

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* TCONPM - Condenser cooling coil temperature (K)
* 10 FT3/MIN * 1 MIN/60 SEC * 0.02832 M3/1 FT3 = 0.00472 M3/SEC
* 2 FT3/MIN * 1 MIN/60 SEC * 0.02832 M3/1 FT3 = 0.000944 M3/SEC
* PUMP IRUPM IROFUM ICONPM ITFZED WPUFUM WPFZED TGFZED
TCONPM 1 3 5 0 0.00472 0.000944 50.00 1.50
* Radiolysis parameters
* FRAD 1.0 ! multiplier for radiolysis
* FALPHA 0.197 ! alpha fractional heat load
* FBETA 0.486 ! beta fractional heat load
* FGAMMA 0.317 ! gamma fractional heat load
* GPHOTO 2.4E-6 ! beta fractional rate in MCO free water per gram
* MUOF 0.0 ! MU of fuel loading
* GENERAL is a comment
END GENERAL
* SOLAR RAD
* pointers to heat sinks representing the cask wall and the top
* solar radiation impinges on these
* IHCASK 42
* IHTOP 44
* look-up table for solar radiation throughout a day (sec vs. W/m2)
* EXTRAPOLATION_TIMDAY PERIOD ! offset by six hours
* 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
* 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
* 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
* 75600.0 79200.0 82800.0 86400.0
* RADSDUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0
* 0.0 0.0 0.0 0.0 0.0 0.0 0.0
END SOLAR_RAD
* FUEL_BSKT 2 ! Total number of fuel baskets
* 1st Fuel Basket
* IHSEL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
* define the heat sinks comprising the first fuel basket (must be
* in pairs, for inner and outer elements)
* IFILNS 0 ! define the adjacent center insert heat sink,
* 0 for no insert
* IFIMCO 15 ! define the adjacent MCO wall heat sink
* IFILID 0 ! define the lid or floor heat sink to which the fuel
* radiates to
* AFIEL 0.131 ! flow area in the basket
* fraction of geometric area exposed for oxidation
* = area available for oxidation/total heat sink area
* 6.8 m2 / (2*33.6 m2) = 0.10119

```

```

* initial amount (kg) of water per geometric surface area (m2) of fuel
* 24 kg / (2*33.6 m2) = 0.3571
* 8.6 kg / (2*33.6 m2) = 0.1271
* FUEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
* FUEL1 0.0 ! on the outer surface of the insert
* FUEL2 0.0 ! on the outer surface of the MCO wall
* FUEL3 0.0 ! on the outer surface of the fuel surface
* FUEL4 0.0 ! wetted fraction of MCO wall
* FUEL5 0.0 ! wetted fraction of fuel surface
* FUEL6 45.0 ! mass of sludge particles (kg) in the fuel basket
* FUEL7 22.5 kg per fuel basket x 2 basket = 45 kg
* view factor matrix between the insert,
* outer surface of outer fuel elements,
* and the MCO wall. Thereafter, the dimension of the square matrix is
* = number of fuel rods. If there is no insert, number of fuel
* rods = 1.
* FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000 0.000
* 0.316 0.027 0.316 0.158 0.018 0.009 0.009 0.009 0.000
* 0.176 0.316 0.000 0.167 0.158 0.316 0.167 0.022
* 0.009 0.018 0.334 0.158 0.000 0.018 0.158 0.107
* 0.000 0.018 0.000 0.000 0.158 0.000 0.000 0.208
* 0.000 0.000 0.018 0.167 0.316 0.316 0.048 0.558
* 0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
* gap distance for micro-convection calculation
* XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
* 0.037 0.000 0.037 0.037 0.056 0.056 0.000 0.000
* 0.037 0.037 0.037 0.000 0.037 0.037 0.037 0.090
* 0.056 0.056 0.037 0.000 0.056 0.056 0.037 0.090
* 0.000 0.056 0.000 0.037 0.056 0.000 0.037 0.056
* 0.000 0.000 0.037 0.037 0.037 0.037 0.000 0.043
* 0.000 0.000 0.000 0.090 0.090 0.090 0.043 0.000
END IHSEL for 1st fuel basket
* 2nd Fuel Basket
* heat sink pairs for second fuel basket
* IHSEL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
* IFILNS 0 ! define the adjacent center insert heat sink,
* 0 for no insert
* IFIMCO 30 ! define the adjacent MCO wall heat sink
* IFILID 43 ! define the lid or floor heat sink to which the fuel
* radiates to
* AFIEL 0.131 ! flow area in the basket,
* fraction of geometric area exposed for oxidation

```

FAI/98-40, Rev. 1

A.16 Input File for Radiation Network Validation

```
*****
* radiation network validation
*****
*
*-----*
* CONTROL      1 Major keyword group
*-----*
*****
```

[illegible]

total number of scrap baskets

[illegible]

Date: 12/31/98

A - 102

FAI/98-40, Rev. 1

```

* species mass, and individual species deposited liquid mass require
* a region and gas name
* Note: plot routine can only accept 99 items; can't plot all things.
* So plot all scrap r's but only 5 fuel (plus MCO)
*
PRESSURE 1 1 ! Pressure in MCO
GAS-T 1 1 ! Temperature in MCO
HS-TI 3 1 2 3 ! Scrap 1 + MCO
HS-TO 3 1 2 3 ! Cask, MCO bott & lid
HS-TA 3 1 2 3 ! Fuel 2
END PLOT ! PLOT is a comment
*
* ACTIVE MODELS ! Keyword; MODELS is a comment; 1 = on, 0 = off
IUNC 0 ! Junction flow model
ICFLW 0 ! Counter-current flow model
INSINK 1 ! Heat sinks
ICNDS 0 ! Condensation
IASED 0 ! Aerosol Sedimentation
IIMC 0 ! Aerosol decay
IIMC 0 ! Fog formation
ISRC 0 ! User-defined sources
IMCO 0 ! MCO models
ISENS 0 ! Sensitivity runs
END ACTIVE MODELS ! ACTIVE MODELS is a comment
*
END CONTROL ! End of CONTROL keyword group
*
* VOLUMES 1 ! total number of control volumes
* No more than 5 columns (regions) at a time
*
VOLUME 1 ! E-6
SED AREA 0.000
ELEVATION 0.000
TEMP GAS 800.0
PRESSURE 1.01325
END REGIONS
END REGIONS
*
* Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
*
GASES 1
HELIUM 0.0
STEAM 0.0
XYGEN 0.2
NITROGEN 0.8
WATER 0.0
END GASES
END VOLUMES ! VOLUMES is a comment

```

```

* Keyword; next line is title, title can be any length
* test for conduction in radial coordinates: fixed temperatures
END TITLE ! Anything after END is a comment
*
* TIMING ! Keyword
* START TIME, >0 FOR RESTART RUN
* RESTART FILE IS READ FROM HANSR.RER
* END TIME (Seconds)
* MIN TIMESTEP (Seconds)
* MAX TIMESTEP (Seconds)
*
TIMING 1.00
200.
1.00
5000.
1.00
10000.
1.00
1000.
*
* PRINT INTERVAL (Seconds)
* MIN PLOT INTERVAL (Seconds)
* MAX PLOT INTERVAL WITHOUT PLOT (Seconds)
* RESTART INTERVAL (Seconds)
* FRACTIONAL CHANGE IN T AND P
* FRACTIONAL CHANGE IN AEROSOL MASS
* FRACTIONAL CHANGE FOR PLOTTING
*
PRINT 1.00
2000000.
0.005
0.005
0.003
END TIMING ! TIMING is a comment.
*
* PRINT ! Keyword for printing section
* Printing syntax:
* HS n list - Heat Sink Temperatures, C
*
HS 3 1 2 3
END PRINT ! PRINT is a comment
*
* PLOT ! Keyword for plotting section
* Plotting syntax:
* PRESSURE n rlist - Pressure, Pa
* GAS-T n rlist - Gas Temperature, K
* HS-TI n rlist - Heat Sink Temperature - Inner Surface, K
* HS-TO n rlist - Heat Sink Temperature - Outer Surface, K
* HS-TA n rlist - Heat Sink Temperature - Average, K
* AEROSOL n rlist - Aerosol Mass (kg), kg
* IMC n rlist - Aerosol Decay, kg/s
* IMC n rlist - Counter-Current Mass Flowrate, kg/s
* GAS-X n rlist - Gas Mole Fraction
* GASNAME n rlist - Gas Name (Species), kg
* GAS-RH n rlist - Gas Relative Humidity
* GAS-MASS n rlist - Gas Mass (Species), kg
* AER-MASS n rlist - Aerosol Mass (Species), kg
* MASS n rlist - Total Mass (Species), kg
* LIQ-MASS n rlist - Deposited Mass (Species), kg
*
* Pressure, Gas Temperature, and total aerosol mass require a region
* list
*
* Heat Sink Temperatures need a heat sink number list
*
* Flowrates need a junction number list
*
* Gas concentration, relative humidity, individual species gas mass,
* individual species aerosol mass, total (gas+aerosol) individual

```

Date: 12/31/98

A - 103

FAI/98-40, Rev. 1

```

*
* rad_network      1      2      3
* fwiqwha         0.0    0.39  0.61
*                0.26  0.33  0.41
*                0.28  0.28  0.44
*
* END HEAT SINKS ! HEAT_SINKS is a comment

```

A.17 Input File for Energy Balance Validation

```

*****
*
* Syntax:
* IGEOM      1 for plane, 0 or 2 for cylinder
* RHO        1000.0 (kg/m3)
* K          100.0 (W/m/K)
* CPHS      500.00 (J/kg/K)
* QV        0.0000 Volumetric Heat Generation (W/m3)
* XRI       0.00000 Inner Radius (m)
* XRO       0.00000 Outer Radius (m)
* AHS       0.00000 One-sided heat sink area (m2)
* TINIT     10.0000 Initial inside surface temperature (C)
* TOUTIT    10.0000 Initial outside surface temperature (C)
* INSULAB   0.0000 Number of insulation layers (1 is minimum)
* IREQI     0.0000 Region index for inner surface or 0 (insulated)
* TIHS      0.0000 Region surface temperature when IREQI = -1 (C)
* IREGO     0.0000 Region index for outer surface or 0 (insulated)
* TOHS      10.0000 Region surface temperature when IREGO = -1 (C)
* XLHS      10.0000 Characteristic length for natural convection (m)
* EHSI      0.0000 Emissivity of inner surface
* EHSO      0.0000 Emissivity of outer surface
*
* SINKS      1      2      3
* IGEOM      1      1      1
* RHO        1000.0 1000.0 1000.0
* K          100.0  50.0   8.0
* CPHS      500.00 500.0 500.0
* QV        0.000 0.000 0.000
* XRI       0.00000 0.0    0.0
* XRO       0.10000 0.1    0.1
* AHS       10.0000 15.000 12.000
* TINIT     10.000 12.000 10.000
* TOUTIT    10.000 12.000 10.000
* INSULAB   0.000 0.000 0.000
* IREQI     0.000 0.000 0.000
* TIHS      10.000 12.000 10.000
* IREGO     0.000 0.000 0.000
* TOHS      10.000 12.000 10.000
* XLHS      1.000 1.000 1.000
* XZHS      0.000 0.000 0.000
* EHSI      0.000 0.000 0.000
* EHSO      0.000 0.000 0.000
*
* STEADY STATE WITH DECAY HEAT
* UNLESS OTHERWISE NOTED, MKS UNITS
*
* GENERAL INPUTS:
* - FIVE TERS OF FUEL PLUS SCRAP EXPLICITLY MODELED
* - VACUUM FLOW RATE IS 35 CFM
* - HE INJECTION IS 1.6 CFM
* - 1.5 KG H2O ON SCRAP BASKET,
* - THIS IS A CONSISTENT PER BASKET ANALYSIS WITH PREVIOUS CALCS,
* - AND IT ALLOWS RESPONSE OF AN EARLY-DRYING BASKET TO BE SEEN.
* - 1.0 KG OF FUEL PER BASKET DIVIDED INTO FINE AND COARSE SECTIONS, WITH
* - RADIAL CONDUCTION TO THE COPPER DIVIDER "FIN"
* - RUN TO ONE DAY
* - AMBIENT TEMPERATURE (CASK EXTERIOR) IS 80 F (26.7 C)
* - CASK/MCO GAP IS 0.61 INCH (0.015 M)
* - BOTH SIDES OF THE CASK AND MCO SURFACE OF MCO WALL TEMPERATURES
* - ARE THE SAME AS THE CASK AND MCO SURFACE OF CASK SURFACE TEMPERATURE. FOR
* - THESE CALCULATIONS, THE CASK AND MCO SURFACE TEMPERATURES ARE
* - THE SAME AS THE CASK AND MCO SURFACE TEMPERATURE. FOR
* - THE CASK HAS INNER DIAMETER OF 25.19" AND OUTER DIAMETER OF
* - 39.81"
* - "WATER" GAS IN THE MCO/CASK GAP
* - "RADIATION HEAT TRANSFER FROM FUEL/SCRAP TO LID/FLOOR."
*
* CONTROL      1 Major keyword group
*
* TITLE        ! Keyword; next line is title, title can be any length
* END TITLE    ! Anything after END is a comment
*
* TIMING       ! Keyword
* TSTART       ! START TIME, >0 FOR RESTART RUN

```

```

* RESTART FILE IS READ FROM HANSF.RER
* END TIME (Seconds)
* MIN TIMESTEP (Seconds)
* MAX TIMESTEP (Seconds)
* PRINT INTERVAL (Seconds)
* MIN PLOT INTERVAL (Seconds)
* MAX PLOT INTERVAL WITHOUT PLOT (Seconds)
* RESTART INTERVAL (Seconds)
* FRACTIONAL CHANGE IN AEROSOL MASS
* FRACTIONAL CHANGE FOR PLOTTING
* END TIMING ! Timing is a comment.

* PLOT
* Keyword for plotting section
* Plotting syntax:
* PRESSURE n rlist - Pressure, Pa
* HS-TI n rlist - Gas Temperature, K
* HS-TI n rlist - Heat Sink Temperature - Inner Surface, K
* HS-TI n rlist - Heat Sink Temperature - Outer Surface, K
* HS-TA n rlist - Heat Sink Temperature - Average, K
* AEROSOL n rlist - Aerosol Mass (Total), kg
* GAS-W n rlist - Mass Flowrate, kg/s
* GAS-WX n rlist - CounterCurrent Mass Flowrate, kg/s
* GAS-X GASNAME n rlist - Gas Mole Fraction
* GAS-RH GASNAME n rlist - Gas Mass (Species), kg
* GAS-MASS GASNAME n rlist - Aerosol Mass (Species), kg
* LIQ-MASS GASNAME n rlist - Deposited Mass (Species), kg
* MASS GASNAME n rlist - Total Mass (Species), kg
* LIQ-MASS GASNAME n rlist - Deposited Mass (Species), kg
* Pressure, Gas Temperature, and total aerosol mass require a region
* list
* Heat Sink Temperatures need a heat sink number list
* Flowrates need a junction number list
* Gas concentration, relative humidity, individual species gas mass,
* individual species aerosol mass, total (gas+aerosol), individual
* species mass, and individual species deposited liquid mass require
* a region and gas name
* Note: Plot routine can only accept 99 items; can't plot all things.
* So plot all scrap T's but only 5 fuel (plus MCO)

PRESSURE 1 1
GAS-T 5 1 2 3 4 5
HS-TI 5 61 62 63 64 65
HS-TI 6 56 67 68 69 70 71
HS-TI 3 72 73 74
HS-O 6 1 4 7 10 14 15
HS-TA 6 1 4 7 10 14 15

```

```

* HS-TA 6 16 19 22 25 29 30
* HS-TA 6 31 34 37 40 44 45
* HS-TA 6 46 49 52 55 59 60
* GAS-X NITROGEN 5 1 2 3 4 5
* GAS-X OXYGEN 5 1 2 3 4 5
* GAS-X STEAM 5 1 2 3 4 5
* GAS-X HYDROGEN 5 1 2 3 4 5
* GAS-X HELIUM 5 1 2 3 4 5
* GAS-W 5 1 2 3 4 5
* GAS-WX 5 1 2 3 4 5
* GAS-MASS HYDROGEN 1 7
* GAS-MASS STEAM 1 7
* END PLOT ! PLOT is a comment

* ACTIVE MODELS ! Keyword; MODELS is a comment; 1 = on, 0 = off
* JUNC 0 ! Junction flow model
* ICFLOW 0 ! Counter-current flow model
* ITHINK 1 ! Heat sink
* ICNDS 0 ! Condensation
* IASED 0 ! Aerosol sedimentation
* ITHINK 0 ! Aerosol packaging
* IFIX 0 ! Fog formation
* ISRC 0 ! User-defined sources
* IMCO 1 ! MCO models
* ISNS 0 ! Sensitivity runs
* END ACTIVE MODELS ! ACTIVE MODELS is a comment

* SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
* END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
* ENTER: TIME, TEMP, FLOWRATES, POWER
* SINTAX EXAMPLE:
* 1.6 FT3/MIN * 1 MIN/60 SEC = 0.0267 M3/1 FT3 = 0.000755 M3/SEC
* 0.0267 M3/1 MIN/60 SEC = 0.000445 M3/1 FT3 = 0.00118 M3/SEC
* Gas density 8 step is 0.16 kg/m3, hence 1.88e-4 about 1.2e-4 kg/s
* Gas density 8 step is 0.16 kg/m3, hence 1.88e-4 about 1.9e-4 kg/s
* He density 8 step is 0.16 kg/m3, hence 1.88e-4 about 1.9e-4 kg/s
* SOURCES 1
* 1 -- KEYWORD AND # SOURCE GROUPS
* REGION 5 GASES 1
* 1 -- REGION #, # GASES
* HELIUM 0 26.85 1.2E-4 0.E0
* 1.86 26.85 1.2E-4 0.E0
* END REGION
* END SOURCE

* END CONTROL ! End of CONTROL keyword group

* VOLUMES 7 ! total number of control volumes
* total MCO gas volume is 0.55 m3, 0.55/3=0.183 per each node
* No more than 5 columns (regions) at a time
* Units!
* VOLUME m3, SED_AREA m2, ELEVATION m, TEMP_GAS C, PRESSURE Pa

```

A - 105

or -1 for constant temperature										MCO WALL									
Region surface temperature when IREGO = -1 (C)																			
Characteristic length for natural convection (m)																			
Emissivity of inner surface																			
Emissivity of outer surface																			
Areas when there were two tiers per fuel basket 1-5,6-10,11-15:																			
AHS 0.557 1.310 0.557 1.310 0.557																			
AHS 1.310 1.114 2.620 0.557 1.310																			
AHS 1.310 1.114 2.620 0.557 1.310																			
Fuel Basket #2 heat sinks 1 through 15																			
SINKS 1 2 3 4 5																			
 																			

Fuel Basket #4 heat sinks 31 through 45									
SINKS	31	32	33	34	35	36	37	38	39
* SINKS	0	0	0	0	0	0	0	0	0
IGEOM	17102.	17102.	17102.	17102.	17102.	17102.	17102.	17102.	17102.
RHO	26.9	26.9	26.9	26.9	26.9	26.9	26.9	26.9	26.9
IRREG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IRGO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	130.00	130.00	130.00	130.00	130.00	130.00	130.00	130.00	130.00
QV	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00
XHS	0.663	0.663	0.663	0.663	0.663	0.663	0.663	0.663	0.663
XRI	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625
Fuel Basket #1 heat sinks 46 through 60									
SINKS	46	47	48	49	50	51	52	53	54
* SINKS	0	0	0	0	0	0	0	0	0
IGEOM	17102.	17102.	17102.	17102.	17102.	17102.	17102.	17102.	17102.
RHO	26.9	26.9	26.9	26.9	26.9	26.9	26.9	26.9	26.9
IRREG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IRGO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPHS	130.00	130.00	130.00	130.00	130.00	130.00	130.00	130.00	130.00
QV	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00	1957.00
XHS	0.663	0.663	0.663	0.663	0.663	0.663	0.663	0.663	0.663
XRI	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610	0.00610
EHSD	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
END	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625	0.01625

Date: 12/31/98

A - 110

DHHV3 3.70E6 ! Decomposition enthalpy J/kg H2O: 3rd step
 FPROHY 1.0 ! hydride production rate law multiplier
 FCONHY 1.0 ! hydride consumption rate law multiplier
 FNTRI 1.0 ! nitriding rate law multiplier
 * PUMP, FEED, AND CONDENSER MODELS
 * PUMP IRUPM IRUPM ICONPM ITFEED WVPUMP WVFEE TGFEE TCONPM
 * SYNTH
 * Definitions:
 IRUPM - Pump inlet region
 IRUPM - Pump outlet region
 ICONPM - Node to which the condensed steam is dumped for back-keeping
 ITFEED - If non-zero, overrides TGFEE with the designated region
 WVPUMP - Pump volumetric flowrate (m³/s)
 WVFEE - Feed volumetric flowrate (m³/s)
 TGFEE - Feed temperature (C)
 TCONPM - Condenser cooling coil temperature (C)
 * 35 FT³/MIN * 1 MIN/60 SEC * 0.0282 M³/1 FT³ = 0.01652 M³/SEC
 * PUMP IRUPM IRUPM ICONPM ITFEED WVPUMP WVFEE TGFEE TCONPM
 * PUMP 1 7 0 0 1.652E-2 0.0 0.0
 * Radiolysis parameters
 * FRAD 1.0 ! multiplier for radiolysis
 * FALPHA 0.197 ! alpha fractional heat load
 * FBETA 0.486 ! beta fractional heat load
 * FGAMMA 0.317 ! gamma fractional heat load
 * OPHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
 * ! percent of total heat loading
 * ! GENERAL is a comment
 * END GENERAL
 * SOLAR_RAD
 * ! pointers to heat sinks representing the cask wall and the top
 * ! solar radiation impinges on these
 * IHCAK 72
 * IHTOP 74
 * Look-up table for solar radiation throughout a day (sec .vs. W/m²)
 * OFFSET TMDAY 21600. ! offset by six hours
 * EXTRAPOLATION PERIOD ! repeat the diurnal cycle
 * TMDAY 0.0 3600.0 7200.0 10800.0 14400.0 18000.0 21600.0
 * 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0
 * 50400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0
 * 75600.0 79200.0 82800.0 86400.0
 * RAD SUN 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 * END SOLAR_RAD
 * FUEL_BSKT 4 ! Total number of fuel baskets

ILAW 1 ! oxidation rate law, 0 - McGillivray/Ritchie
 ! ! Reactor core due to scrap basket
 IDEENT 0 ! de-entrainment of sludge to scrap basket
 ! ! de-entrainment calculation
 IENTR 0 ! de-entrainment of sludge particle calculation
 ! ! de-entrainment calculation
 IENHRA 0 ! de-entrainment of fuel oxide hydrate
 ! ! de-entrainment calculation
 INTRI 0 ! de-entrainment of nitriding calculation
 ! ! de-entrainment calculation
 IRADDO 0 ! de-entrainment of radiolysis calculation
 ! ! de-entrainment calculation
 IHSKSK 2,E-5 ! average diameter of sludge particle (m)
 ! ! de-entrainment calculation
 IRGAP 7 ! define the gap node (between MCO wall and the cask)
 ! ! radiative/convective h.t. between the MCO wall and
 ! ! the cask is computed and some of the heat is
 ! ! goes for stability
 ! ! gap distance between the MCO wall and the cask
 XGFSK 0.0155 ! fuel/scraper for the radiative heat transfer between the
 FHTLID 1.0 ! fuel/scraper for the radiative heat transfer
 ! ! fuel/scraper for the radiative heat transfer
 RHUOL 5000. ! sludge particle density (kg/m³)
 SASL 1000. ! sludge specific area (m²/m³)
 XDLSL 1,E-6 ! sludge particle diameter (m)
 * Hydrate Model: two-step decomposition,
 * input curves for ln P and ln K
 * first step for x > XHYD1, second step for x < XHYD2
 * Bounding cases: 42 kg particulate, 0.8 kg h2o = 1.9%
 * water per mole of uranium oxide
 * FHYSL 0.1732 ! fraction of sludge that is hydrated
 XHYSL 2.0 ! stoichiometry number of hydrate: UO3.H2O
 XHYD2 1.0 ! H2O/U ratio (second correlation)
 XHYD3 0.5 ! H2O/U ratio (stoich. number) to switch
 ! ! from second to third correlation
 * ANHYEQ1 15.912 ! 'A' IN LN P = A + B/T FOR X > XHYD2
 ! 'B' IN LN P = A + B/T FOR X > XHYD2
 ANHYEQ2 -6131.50 ! 'A' IN LN P = A + B/T FOR X < XHYD2
 ! 'B' IN LN P = A + B/T FOR X < XHYD2
 ANHYEQ3 -19.382 ! 'A' IN LN P = A + B/T FOR X < XHYD2
 ! 'B' IN LN P = A + B/T FOR X < XHYD2
 ANHYEQ4 -7766.80 ! 'A' IN LN P = A + B/T FOR X < XHYD2
 ! 'B' IN LN P = A + B/T FOR X < XHYD2
 ANHYEQ5 -18.408 ! 'A' IN LN P = A + B/T FOR X < XHYD2
 ! 'B' IN LN P = A + B/T FOR X < XHYD2
 ANHYEQ6 -8488.20 ! 'A' IN LN P = A + B/T FOR X < XHYD2
 ! 'B' IN LN P = A + B/T FOR X < XHYD2
 * ANHYEQ7 2.79320 ! 'A' IN LN K = A + B/T FOR X > XHYD2
 ! 'B' IN LN K = A + B/T FOR X > XHYD2
 ANHYEQ8 -5111.50 ! 'A' IN LN K = A + B/T FOR X < XHYD2
 ! 'B' IN LN K = A + B/T FOR X < XHYD2
 ANHYEQ9 6.34880 ! 'A' IN LN K = A + B/T FOR X < XHYD2
 ! 'B' IN LN K = A + B/T FOR X < XHYD2
 ANHYEQ10 -7241.80 ! 'A' IN LN K = A + B/T FOR X < XHYD2
 ! 'B' IN LN K = A + B/T FOR X < XHYD2
 ANHYEQ11 4.63220 ! 'A' IN LN K = A + B/T FOR X < XHYD2
 ! 'B' IN LN K = A + B/T FOR X < XHYD2
 ANHYEQ12 -7548.50 ! 'A' IN LN K = A + B/T FOR X < XHYD2
 ! 'B' IN LN K = A + B/T FOR X < XHYD2
 * DHHV1 2.865E ! Decomposition enthalpy J/kg H2O: 1st step
 DHHV2 3.705E ! Decomposition enthalpy J/kg H2O: 2nd step

FAI/98-40, Rev. 1

Date: 12/31/98

A - 111

```

* * gap distance for micro-convection calculation
* *
* * XGAP 0.000 0.021 0.021 0.073 0.000 0.000 0.000 0.000 0.000
* *
* * IHSEL 46 47 48 49 50 51 52 53 54 55 56 57 58 59
* * ! define the adjacent center insert heat sink,
* * IFILNS 0 ! 0 for no insert
* * IFMCO 60 ! define the adjacent MCO wall heat sink
* * IFILFD 0 ! define the lid or floor heat sink to which the fuel
* * ! elicits to
* * AFELF 0.131 ! flow area in the basket,
* *
* * 2nd Fuel Basket
* *
* * IHSEL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
* * ! define the heat sinks comprising the first fuel basket (must be
* * ! in pairs, for inner and outer elements)
* *
* * IFILNS 0 ! define the adjacent center insert heat sink,
* * IFMCO 15 ! define the adjacent MCO wall heat sink
* * IFILFD 0 ! define the lid or floor heat sink to which the fuel
* * ! elicits to
* * AFELF 0.131 ! flow area in the basket
* *
* * ! fraction of geometric area exposed for oxidation
* * ! 3.5 m2 / (4*16.8 m2) = 0.0521
* * FROXFL 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521
* * FOX 10 0 ! multiplier for FROXFL
* *
* * ! Nominal hydride: 4% of exposed surface with multiplier of 300
* * ! XFLXO*FXHD0 = FX * Fa * XDHYD / 6, where Fa is area fraction
* * ! = 0.04 * 300 * 2.E-5 / 6
* * ! = 4.0E-5
* *
* * XFLXO: initial oxide (oxide+hydride) thickness
* * FXHD0: fraction of initial oxide which is hydride
* *
* * XFLXO 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
* * 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
* * FXHD0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
* *
* * ! initial amount (kg) of water per geometric surface area (m2) of fuel
* * ! FWELO kg (1.0 m2 of water per geometric surface area (m2) of fuel
* * FWELO 0.0060 0.0060 0.0060 0.0060 0.0060 0.0060 0.0060
* * FWELO 0.0 ! on the outer surface of the insert
* * FWELO 0.0 ! on the inner surface of the MCO wall
* * FWELO 0.1 ! wetted fraction of fuel surface
* * FWELO 1.0 ! wetted fraction of MCO wall
* * MSLEFL 5.2 ! mass of sludge particles (kg) in the fuel basket
* * ! 20.8 total fuel # 4 baskets, so 5.2 per basket
* *
* * ! view factor matrix between the insert,
* * ! outer surface of outer fuel elements,
* * ! and the MCO wall. Therefore, the dimension of the square matrix is
* * ! 1*number of fuel rods+1. If there is no insert, number of fuel
* * ! rods+1.
* *
* * FVIEW 0.473 0.320 0.181 0.028 0.000 0.000 0.000 0.000
* * 0.320 0.306 0.306 0.028 0.014 0.000 0.000 0.000
* * 0.181 0.306 0.306 0.028 0.014 0.000 0.000 0.000
* * 0.028 0.014 0.153 0.167 0.153 0.000 0.028 0.028
* * 0.014 0.153 0.167 0.153 0.153 0.000 0.028 0.028
* * 0.000 0.014 0.000 0.028 0.028 0.000 0.306 0.348
* * 0.000 0.000 0.014 0.000 0.306 0.028 0.000 0.306
* * 0.000 0.000 0.014 0.167 0.153 0.153 0.049 0.466
* * 0.000 0.000 0.000 0.035 0.115 0.220 0.590 0.040

```

FAI/98-40, Rev. 1

```
* initial amount (kg) of water per geometric surface area (m2) of fuel
* 6 kg / (16.8 m2) = 0.3571
FWFLZ0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
FWFLZ1 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
FWFLZ2 0.0 ! on the outer surface of the MCO wall
FWFLZ3 0.0 ! on the inner surface of the MCO wall
FWFLZ4 0.0 ! wetted fraction of fuel surface
FWFEL0 0.1 ! wetted fraction of fuel surface
FWFEL1 0.1 ! wetted fraction of fuel surface
FWFEL2 0.1 ! wetted fraction of fuel surface
FWFEL3 0.1 ! wetted fraction of fuel surface
HSHSL 5.2 ! number of hydrogen particles (kg) in the fuel basket
! 20.8 total fuel & 4 baskets, so 5.2 per basket

** view factor matrix between the insert,
** outer surface of outer fuel elements,
** and the MCO wall. Therefore, if there is no insert, number of fuel rods=1.
FVIEW      0.473   0.320   0.181   0.028   0.000   0.000   0.000   0.000
          0.320   0.028   0.306   0.306   0.028   0.014   0.000   0.000
          0.181   0.306   0.000   0.334   0.153   0.000   0.028   0.000
          0.014   0.153   0.167   0.167   0.133   0.000   0.167   0.028
          0.000   0.028   0.153   0.306   0.009   0.028   0.306   0.133
          0.000   0.014   0.000   0.306   0.028   0.153   0.009   0.466
          0.000   0.000   0.000   0.000   0.028   0.153   0.049   0.466
          0.000   0.000   0.000   0.035   0.115   0.220   0.590   0.040

** gap distance for micro-convection calculation
XGAP      0.000   0.021   0.021   0.073   0.000   0.000   0.000   0.000
          0.021   0.000   0.021   0.021   0.073   0.073   0.073   0.000
          0.021   0.021   0.000   0.021   0.021   0.073   0.073   0.000
          0.000   0.073   0.021   0.021   0.021   0.021   0.083   0.083
          0.000   0.073   0.000   0.021   0.000   0.073   0.021   0.058
          0.000   0.000   0.073   0.000   0.021   0.073   0.000   0.021
          0.000   0.000   0.000   0.073   0.021   0.021   0.000   0.016
          0.000   0.000   0.000   0.000   0.083   0.058   0.026   0.016

END IHSEFL for 3rd fuel basket

** 4th Fuel Basket
IHSEFL    31 32 33 34 35 36 37 38 39 40 41 42 43 44
** define the heat sinks comprising the first fuel basket (must be
** in pairs, for inner and outer elements)
IFILNS 0 ! define the adjacent center Insert heat sink,
         0 for no insert
IFLMCO 45 ! define the adjacent MCO wall heat sink
IFILLD 75 ! define the lid or floor heat sink to which the fuel
           radiates to
AFLEFL 0.131 ! flow area in the basket

** fraction of geometric area exposed for oxidation
FX 3.5 m2 / ((4*16.8 m2) - 0.0521)
FAOXFL 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521
FOX     10 0 ! multiplier for FPAOXL

** Nominal hydrides: 4% of exposed surface with multiplier of 300
XFLOXH=FHHDD = FX * FX * XHDWD / 6, where FX is multiplier
```

Date: 12/31/98

* outer surface of outer fuel elements,
* and the MCO wall. Therefore, the dimension of the square matrix is
* =number of fuel rods+1. If there is no insert, number of fuel
* rods=1.
FVIEW 0.473 0.326 0.181 0.098 0.000 0.000 0.000 0.000
0.151 0.306 0.162 0.086 0.028 0.014 0.000 0.000
0.014 0.153 0.167 0.334 0.153 0.053 0.028 0.000
0.000 0.028 0.153 0.306 0.153 0.153 0.153 0.028
0.000 0.014 0.000 0.306 0.000 0.028 0.306 0.181
0.000 0.000 0.014 0.157 0.306 0.028 0.000 0.348
0.000 0.000 0.014 0.157 0.153 0.153 0.049 0.466
0.000 0.000 0.000 0.035 0.115 0.220 0.590 0.040
* gap distance for micro-convection calculation
XGAP 0.000 0.021 0.021 0.073 0.000 0.000 0.000 0.000
0.021 0.000 0.021 0.021 0.073 0.073 0.000 0.000
0.021 0.021 0.000 0.021 0.021 0.000 0.073 0.000
0.073 0.021 0.021 0.000 0.021 0.021 0.000 0.083
0.000 0.073 0.021 0.021 0.000 0.073 0.021 0.056
0.000 0.073 0.000 0.021 0.073 0.021 0.000 0.016
0.000 0.000 0.000 0.000 0.083 0.058 0.026 0.016
END IHSEFL for 2nd fuel basket
* 3rd Fuel Basket
* heat sink pairs for second fuel basket
IHSFPL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
IFLINS 0 : define the adjacent center insert heat sink,
0 : for no insert
IFLMCO 30 : define the adjacent MCO wall heat sink
IFLLD 0 : define the lid or floor heat sink to which the fuel
radiate to
AFLFL 0.131 : flow area in the basket,
* fraction of geometric areas exposed for oxidation
FAOXE 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521
FXOFL 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521 0.0521
FOX 10 0 : multiplier for FMOXFL
* Nominal hydride: 4% of exposed surface with multiplier of 300
* XFLOXO*FXHDD = FX * Fa * XHDHY / %, where Fa is multiplier
* of initial oxide thickness and Fa is area fraction
= 0.04 * 300 * 2.E-5 / %
= 4.0E-5
* XFLOXO: initial oxide (oxide+hydride) thickness
(to be applied to exposed area)
* FXHDD: fraction of initial oxide which is hydride
XFLOXO 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
FXHDD 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0

A - 112

FAI/98-40, Rev. 1

A - 113

FAI/98-40, Rev. 1

APPENDIX B
SAMPLE PROBLEM INPUT

IFOG 0 ! Fog formation
 IESC 1 ! User-defined sources
 IMCO 1 ! MCO models
 ISNS 0 ! Sensitivity runs
 END ACTIVE MODELS ! ACTIVE MODELS is a comment
 END

* If there are more than five regions, continue here.

* GASES 1 2 3 4 5
 HELIUM 0.89 0.89 0.0 0.0
 STEAM 0.11 0.11 0.0 0.0
 OXYGEN 0.0 0.0 0.0 0.0
 NITROGEN 0.0 0.0 0.0 0.0
 WATER 0.0 0.0 0.0 1.0
 END GASES ! GASES is a comment

* If there are more than five regions, continue here.

* GASES 6 7
 HELIUM 0.89 0.0
 STEAM 0.11 0.0158
 OXYGEN 0.0 0.0
 NITROGEN 0.0 0.7775
 WATER 0.0 0.0
 END GASES ! GASES is a comment

* Aerosol concentration of each region (kg/m³)
 * No more than five columns at a time
 * AEROSOLS 1 2 3 4 5
 STEAM 0.0001 0.0 0.0 0.0
 END AEROSOLS ! AEROSOLS is a comment

* No more than five columns at a time, so continue with 6 & 7

* AEROSOLS 6 7
 STEAM 0.0 0.0
 END AEROSOLS ! AEROSOLS is a comment

* OPTIONAL TEMPERATURE AND PRESSURE CONTROL
 * CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
 * IMPOSE TEMPERATURE LOOK-UP TABLE
 * SYNTAX: TIMEG= OFFSET TIMEG
 * EXTRAPOLATION TIMEG
 * TIMEG IREG TIME1, TIME2... TIMELAST
 * TGFIX IREG TIME1, TIME2... TIMEPLAST
 * LINEAR INTERPOLATION BETWEEN VALUES
 * SIMILAR SYNTAX FOR PRESSURE:
 * OFFSET TIMEG
 * EXTRAPOLATION TIMEG
 * TIMEP IREG TIME1, TIME2...
 * PFIIX IREG PRES1, PRES2...
 * PRESSURES ARE IN PAII
 * OFFSET TIMEG= OFFSET TIME; ENTER LOOKUP TABLE WITH
 * EXTRAPOLATION TIMEG= TIME-OFFSET TIMEG
 * EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
 * - PERIOD TO WANT AROUND.
 * OFFSET TIMEG 50.
 * EXTRAPOLATION TIMEG LAST
 * TIMEG 1 0.0 100. 200.
 * TGFIX 1 293.15 373.15 473.15
 * CONTROL MCO BOUNDARY P, 30.
 * OFFSET TIMEG

Date: 12/31/98

B-3

IFOG 0 ! Fog formation
 IESC 1 ! User-defined sources
 IMCO 1 ! MCO models
 ISNS 0 ! Sensitivity runs
 END ACTIVE MODELS ! ACTIVE MODELS is a comment
 END

* If there are more than five regions, continue here.

* SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
 * END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
 * ENTER: TIME, TEMP, FLOWRATES, POWER
 * SYNTAX EXAMPLE:
 * SOURCES 1
 * !--- KEYWORD AND # SOURCE GROUPS
 * !--- REGION # GASES
 * !--- GAS NAMES MUST BE ON NEXT LINE
 * REGION 3 GASES 1
 * HELIUM
 * 0 30.0 1.9E-4 0.20
 * 1.1E 30.0 1.9E-4 0.20
 * !--- ENDS A REGION SOURCE
 * END REGION
 * END SOURCE
 * END CONTROL ! End of CONTROL keyword group

* VOLUMES 5 ! total number of control volumes
 * total MCO gas volume is 0.55 m³, 0.55/3=0.183 per each node
 * No more than 5 columns (regions) at a time
 * VOLUME m³, SED_AREA m², ELEVATION m, TEMP_GAS K, PRESSURE Pa
 * MCO top MCO middle MCO bottom gap environment

REGIONS 1 2 3 4 5
 VOLUME 0.100 0.200 0.200 0.25 1.19
 SED_AREA 0.172 0.172 0.172 0.0 0.0
 ELEVATION 2.65 1.33 0.0 0.0 0.0
 TEMP_GAS 50.0 50.0 50.0 50.0 50.0
 PRESSURE 1.0135 1.0135 1.0135 1.0135 1.0135
 END REGIONS ! REGIONS is a comment

* If there are more than five regions, continue here.

* REGIONS 6 7
 VOLUME 1.19 0.0
 SED_AREA 0.27 0.0
 ELEVATION 0.0 0.0
 TEMP_GAS 323.15 299.85
 PRESSURE 1.0475 1.0475
 END REGIONS ! REGIONS is a comment

* Gas composition of each region; specify mole fraction of each gas
 * No more than five columns at a time

1/1/98-40, Rev. 1

Date: 12/31/98

B-6

1 20.8 total fuel, no 10.4 per basket pair

* view factor matrix between the insert,
* outer surface of outer fuel elements,
* and the MCO wall. Therefore, the dimension of the square matrix is
* 1 number of fuel rods+1. If there is no insert, number of fuel
* rods+1.

FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000 0.000
0.316 0.027 0.000 0.167 0.058 0.009 0.009 0.000 0.000
0.176 0.000 0.000 0.167 0.158 0.000 0.009 0.009 0.000
0.009 0.316 0.334 0.167 0.316 0.316 0.316 0.167 0.022
0.000 0.018 0.158 0.158 0.000 0.018 0.158 0.107
0.000 0.009 0.000 0.158 0.018 0.000 0.158 0.208
0.000 0.000 0.018 0.167 0.316 0.316 0.048 0.558
0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106

* gap distance for micro-convection calculation

* KGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.000 0.037 0.037 0.056 0.056 0.000 0.000
0.037 0.037 0.000 0.037 0.037 0.037 0.037 0.000
0.056 0.037 0.037 0.000 0.037 0.037 0.037 0.090
0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.090
0.000 0.056 0.000 0.037 0.056 0.000 0.037 0.056
0.000 0.000 0.037 0.037 0.037 0.000 0.043
0.000 0.000 0.000 0.037 0.037 0.037 0.043 0.000

END IHSELF for 1st fuel basket

* 2nd Fuel Basket

* heat sink pairs for second fuel basket

THSELF 16 17 18 19 20 21 22 23 24 25 26 27 28 29
IFLINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
IFLMCO 30 ! define the adjacent MCO wall heat sink
IFLFLD 43 ! define the lid or floor heat sink to which the fuel
! radiate to

AFLEFL 0.131 ! flow area in the basket,
! fraction of geometric area exposed for oxidation
FXMCO² / (2*33.6 m²) = 0.10417
FXMFL² / (2*33.6 m²) = 0.10417
FXMFL 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417
FOX 10 0 ! multiplier for FANFL

* Nominal hydride: 4.0% of exposed surface with multiplier of 300
* FXELOXO+FXHDO = FX * Fa * XDHYD / 6, where Fa is multiplier
* FXELOXO+FXHDO = FX * Fa * XDHYD / 6, where Fa is area fraction
* = 0.040 * 300 * 2.E-5 / 6
* = 4.0E-5
* FXELOXO: initial oxide (oxide+hydride) thickness
* (to be applied to exposed area)
* FXHDO: fraction of initial oxide which is hydride
FXELOXO 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
FXHDO 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0

* initial amount (kg) of water per geometric surface area of fuel
* 24 kg / (2*33.6 m²) = 0.3571
FXWLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
FXWLO 0.0 ! on the outer surface of the insert
FXWLO 0.4545 ! on the inner surface of the MCO wall
FXWFL 0.1 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall

* initial amount (kg) of water per geometric surface area of fuel
* 24 kg / (2*33.6 m²) = 0.3571
FXWLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
FXWLO 0.0 ! on the outer surface of the insert
FXWLO 0.4545 ! on the inner surface of the MCO wall
FXWFL 0.1 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall

* Water mass and sludge water mass require a heat sink list

* Hydrogen flow rate requires a junction list

PUMPFR2 ! hydrogen pumping flow rate
CORROH2 2 ! hydrogen corrosion rate by corrosion
GAS-RVH2O 2 1 1 mass of water on h.s. 1 & 14
GAS-RVH2O 2 1 1 mass of sludge water on h.s. 1 & 14
H2S-RVH2O 2 1 2 3 ! hydrogen flow rate thru junctions 1, 2, & 3
END PLOT ! PLOT is a comment

FUEL_BSKT 2 ! Total number of fuel baskets

* 1st Fuel Basket

THSELF 1 2 3 4 5 6 7 8 9 10 11 12 13 14
IFLINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
IFLMCO 15 ! define the adjacent MCO wall heat sink
IFLFLD 0 ! define the lid or floor heat sink to which the fuel
! radiate to

AFLEFL 0.131 ! flow area in the basket
! fraction of geometric area exposed for oxidation
FXMCO² / (2*33.6 m²) = 0.10417
FXMFL² / (2*33.6 m²) = 0.10417
FXMFL 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417
FOX 10 0 ! multiplier for FANFL

* Nominal hydride: 4.0% of exposed surface with multiplier of 300
* FXELOXO+FXHDO = FX * Fa * XDHYD / 6, where Fa is multiplier
* FXELOXO+FXHDO = FX * Fa * XDHYD / 6, where Fa is area fraction
* = 0.040 * 300 * 2.E-5 / 6
* = 4.0E-5
* FXELOXO: initial oxide (oxide+hydride) thickness
* (to be applied to exposed area)
* FXHDO: fraction of initial oxide which is hydride
FXELOXO 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
FXHDO 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0

* initial amount (kg) of water per geometric surface area of fuel
* 24 kg / (2*33.6 m²) = 0.3571
FXWLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
FXWLO 0.0 ! on the outer surface of the insert
FXWLO 0.4545 ! on the inner surface of the MCO wall
FXWFL 0.1 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall

* initial amount (kg) of water per geometric surface area of fuel
* 24 kg / (2*33.6 m²) = 0.3571
FXWLO 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
FXWLO 0.0 ! on the outer surface of the insert
FXWLO 0.4545 ! on the inner surface of the MCO wall
FXWFL 0.1 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall
FXWFL 1.0 ! wetted fraction of MCO wall

* Water mass and sludge water mass require a heat sink list

* Hydrogen flow rate requires a junction list

PUMPFR2 ! hydrogen pumping flow rate
CORROH2 2 ! hydrogen corrosion rate by corrosion
GAS-RVH2O 2 1 1 mass of water on h.s. 1 & 14
GAS-RVH2O 2 1 1 mass of sludge water on h.s. 1 & 14
H2S-RVH2O 2 1 2 3 ! hydrogen flow rate thru junctions 1, 2, & 3
END PLOT ! PLOT is a comment

FUEL_BSKT 2 ! Total number of fuel baskets

* 1st Fuel Basket

THSELF 1 2 3 4 5 6 7 8 9 10 11 12 13 14
IFLINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
IFLMCO 15 ! define the adjacent MCO wall heat sink
IFLFLD 0 ! define the lid or floor heat sink to which the fuel
! radiate to

AFLEFL 0.131 ! flow area in the basket
! fraction of geometric area exposed for oxidation
FXMCO² / (2*33.6 m²) = 0.10417
FXMFL² / (2*33.6 m²) = 0.10417
FXMFL 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417
FOX 10 0 ! multiplier for FANFL

* Nominal hydride: 4.0% of exposed surface with multiplier of 300
* FXELOXO+FXHDO = FX * Fa * XDHYD / 6, where Fa is multiplier
* FXELOXO+FXHDO = FX * Fa * XDHYD / 6, where Fa is area fraction
* = 0.040 * 300 * 2.E-5 / 6
* = 4.0E-5
* FXELOXO: initial oxide (oxide+hydride) thickness
* (to be applied to exposed area)
* FXHDO: fraction of initial oxide which is hydride
FXELOXO 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5 4.0E-5
FXHDO 1.0 1.0 1.0

* * * * *

* MCO SHIPPING: AVERAGE MCO 770 W, AVG WATER, BOUNDING RX AREA

* NOMINAL HYDRIDE

* * * * *

* EXPOSED TO MAX SOLAR FLUX, HOT DAY, NOON START, 2 HOUR RUN

* * * * *

* RESTART: 8 HOURS AFTER CVD ANGLIUS DRAIN

* * * * *

* 0.144 KG HYDRATE WATER INVENTORY - BEST EST.

* * * * *

* UNLESS OTHERWISE NOTED, MKS UNITS

* * * * *

* - 1 TIER OF SCHAR BASKET

* - 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)

* * * * *

```
* CONTROL      Major keyword group
**
** TITLE Keyword; next line is title, title can be any length
** SHIPING, NOT DAY, 770 W
** END TITLE ! Anything after END is a comment
** NOMINAL 2 HOURS TO FEED INDOOR STAGING
**
** TITING      Keyword
** START TIME, >0 FOR RESTART RUN
** RESTART FILE IS READ FROM HANSF.RER
** END TIME (Seconds)
** MAX TIMESTEP (Seconds)
** PRINT INTERVAL (Seconds)
** MIN PLOT INTERVAL (Seconds)
** MAX PLOT INTERVAL WITHOUT PLOT (Seconds)
** RESTART INTERVAL (Seconds)
** FRACTIONAL CHANGE IN TH AND P
** FRACTIONAL CHANGE IN AEROSOL MASS
** FRACTIONAL CHANGE FOR PLOTTING
** STOPPING PLOTTING, anything is a comment.
```

```

*
*      ! Keyword for plotting section
*      PLOT
*
*      ! Plotting syntax:
*
*      * PRESSURE n rlist - Pressure, Pa
*      * GAS-T n rlist - Gas Temperature, K
*      * HS-TI n rlist - Heat Sink Temperature - Inner Surface, K
*      * HS-TO n rlist - Heat Sink Temperature - Outer Surface, K
*      * HS-T n rlist - Heat Sink Temperature - Average, K
*      * HS-CG n rlist - Aerocool Mass (Total), kg

```

FAI/98-40, Rev. 1

B - 10

```

C   END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
C   ENTER: TIME, TEMP, TEMP, FLOWRATES, POWER
C   SYNTAX EXAMPLE:
C   SOURCES 2      1--- KEYWORD AND # SOURCE GROUPS
C   REGION 1 GASES 2      1--- REGION #, # GASES
C   STEAM HYDROGEN      1--- GAS NAMES MUST BE ON NEXT LINE
C   0 300 1.E-3 1.E-3 0.20
C   0 300 1.E-3 1.E-3 0.20
C   END REGION      1--- ENDS A REGION SOURCE
C   END SOURCE      1--- ENDS ALL SOURCE INPUT
C   END CONTROL      1 End of CONTROL keyword group
C
C-----
C   VOLUMES 5      1 total number of control volumes
C   Control MCO gas volume is 0.50 m^3; gap is 0.6" & 0.3 m x 4 m
C   No more than 5 columns (regions) at a time
C   VOLUME M^3, SED_AREA M^2, ELEVATION m, TEMP GAS K, PRESSURE Pa
C   Units:
C   REGIONS 1 2 3 4 5
C   VOLUME 0.100 0.200 0.200 0.200 0.02 1.E9
C   SED_AREA 0.172 0.172 0.172 0.0 0.0 0.0
C   ELEVATION 2.65 1.33 0.0 0.0 0.0
C   TEMP GAS 44.31 47.62 49.36 31.57 41.0
C   PRESSURE 1.181E5 1.181E5 1.181E5 1.056E5 1.013E5
C   END REGIONS      1 REGIONS is a comment
C
C   Gas composition of each region; specify mole fraction of each gas
C   No more than five columns at a time
C   GASES 1 2 3 4 5
C   Mole fractions of gas 0.00E+00 0.00E+00 0.00E+00 7.900E-01 7.900E-01
C   NITROGEN 0.000E+00 0.000E+00 0.000E+00 0.000E+00 2.100E-01
C   OXYGEN 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
C   Sulfur 1.40E-05 1.20E-05 1.22E-05 0.000E+00 0.000E+00
C   HYDROGEN 7.08E-02 7.08E-02 7.08E-02 0.000E+00 0.000E+00
C   HELIUM 9.291E-01 9.291E-01 9.292E-01 0.000E+00 0.000E+00
C   END GASES      1 GASES is a comment
C
C   Aerosol concentration of each region (kg/m^3)
C   No more than five columns at a time
C   AEROSOLS 1 2 3 4 5
C   STEAM 0.0001 0.0 0.0 0.0 0.0
C   END AEROSOLS      1 AEROSOLS is a comment
C
C   OPTIONAL TEMPERATURE AND PRESSURE CONTROL
C   CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
C   IMPOSE TEMPERATURE LOOK-UP TABLE
C   SYNTAX:
C   OFFSET_TIMEG

```

```

* EXTRAPOLATION TIMEG
* TIMEG IRG TIME1, TIME2...TIMELAST
* TGFX IRG TEMP1, TEMP2...TEMPLAST
* LINEAR INTERPOLATION BETWEEN VALUES
*
* SIMILAR SYNTAX FOR PRESSURE:
* OFFSET_TIMEG
* EXTRAPOLATION TIMEPG
* TIMEP IRG TIME1, TIME2...
* PREFIX IRG PRES1, PRES2...PRESSURES ARE IN PA!!
*
* OFFSET_TIMEG= TIME-OFFSET TIMEG
* EXTRAPOLATION_TIMEG= LAST TO USE LAST VALUE IN THE TABLE,
* = EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
* = PERIOD TO WRAP AROUND.
*
* TIME-TEMP. TABLE STARTS AT MIDNIGHT. SHIFT RUN TO BEGIN AT NOON:
* NOON = TSTART + OFFSET, SO OFFSET = 12 - 8 = 4 HOURS
*
* OFFSET TIMEG 14.4E3
* EXTRAPOLATION_TIMEG PERIOD
*
* TIMEG 5 0.0 7.2E3 14.4E3 21.6E3 28.8E3 36.0E3 43.2E3
* 50.4E3 57.6E3 64.8E3 72.0E3 79.2E3 86.4E3
*
* TGFX 5 27.75 25.55 23.85 23.34 29.45 36.15 39.45
* 43.85 46.15 45.05 37.75 31.65 27.75
*
* CONTROL MCO BOUNDARY P, 30.
* OFFSET TIMEG EXTRAP
* EXTRAPOLATION TIMEPG EXTRAP
* TIMEP 1 0.0 100. 200.
* PREFIX 1 1.E5 1.2E5 1.4E5
*
* END VOLUMES      1 VOLUMES is a comment
*
* Major keyword-----
* HEAT SINKS 44      1 Total number of heat sinks
*
* decay power based on 835 W per MCO.
* No more than 5 columns at a time,
* Repeat the following structure,
* SINKS
*
* END
*
* Syntax:
* RHO Density (kg/m^3)
* RHO Thermal Conductivity (W/m/K)
* RHO Specific Heat (J/kg/K)
* CVHS Volumetric Heat Generation (W/m^3)
* XRI Inner Radius (m)
* XRO Outer Radius (m); for plane wall, thickness = XRO-XRI
* AHS One-sided heat sink area (m^2)

```


* look-up table for solar radiation throughout a day (sec. vs. W/m²)

* NOON = TSFART + OFFSET, SO OFFSET = 12 - 8 = 4 HOURS

* OFFSET_TMDAY_TMDAY 14 FEB 1 offset by 4 hours

* EXTRAPOLATION_TMDAY PERIOD 1 repeat the diurnal cycle

* TMDAY 0.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0

* 25200.0 28800.0 32400.0 36000.0 39600.0 43200.0 46800.0

* 52400.0 54000.0 57600.0 61200.0 64800.0 68400.0 72000.0

* 75600.0 79200.0 82800.0 86400.0 0 0 0

* RADSDN 0.0 0.0 0.0 0.0 0.0 0.0 0.0

* 47.9 78.1 108.0 131.3 147.7 155.9 155.5

* 146.7 130.9 108.0 80.3 51.1 24.4 6.3

* END SOLAR_RAD 0.0 0.0 0.0 0.0 0.0 0.0 0.0

* FUEL_BSKT 2 1 Total number of fuel baskets

* 1st Fuel Basket

* HSEFL 1 2 3 4 5 6 7 8 9 10 11 12 13 14

* define the heat sinks comprising the first fuel basket (must be

* in pairs, for inner and outer elements)

* IFLINS 0 1 define the adjacent center insert heat sink,

* IFLMCO 15 1 define the adjacent MCO wall heat sink

* IFLILO 0 1 define the lid or floor heat sink to which the fuel

* radiates to

* AFLEFL 0.131 1 flow area in the basket

* fraction of geometric area exposed for oxidation

* area available for oxidation/total heat sink area

* fraction of geometric area exposed for oxidation

* 7.0 m² (2433.6 m²) = 0.10417

* FROMED 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417

* FOX 10.0 0.0 1 multiplier for FOMFL 4.0e-5 4.0e-5 4.0e-5 4.0e-5

* MFLXO 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5

* FMHYD 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5

* 1.0 1.0 1.0 1.0 1.0 1.0 1.0

* initial amount (kg) of water per geometric surface area (m²) of fuel

* 0 kg / (2433.6 m²)

* FFWLO 0.0 0.0 0.0 0.0 0.0 0.0 0.0

* FFWLLO 0.0 0.0 0.0 0.0 0.0 0.0 0.0

* on the outer surface of the insert

* on the inner surface of the MCO wall

* FFWLLO 0.0 1 on the inner surface of the MCO wall

* FFWLLO 0.1 1 wetted fraction of MCO wall

* FFWLLO 1.0 1 wetted fraction of MCO wall

* MSLEFL 1.08 1 mass of sludge particles (kg) in the fuel basket

* view factor matrix between the insert,

* outer surface of outer fuel elements,

* and the MCO wall. Therefore, the dimension of the square matrix is

* ARHEQ1 15.912 1 'A' IN LN P = A + B/T FOR X > XHVD2

* SHVEQ1 -6131.E0 1 'B' IN LN P = A + B/T FOR X > XHVD2

* ARHEQ2 15.912 1 'A' IN LN P = A + B/T FOR X < XHVD1

* SHVEQ2 -6131.E0 1 'B' IN LN P = A + B/T FOR X < XHVD1

* ARHEQ3 -18.408 1 'A' IN LN P = A + B/T FOR X > XHVD3

* SHVEQ3 -8468.E0 1 'B' IN LN P = A + B/T FOR X > XHVD3

* ADEHY1 2.793E0 1 'A' IN LN K = A + B/T FOR X > XHVD2

* SDEHY1 -5111.E0 1 'B' IN LN K = A + B/T FOR X > XHVD2

* ADEHY2 6.348E0 1 'A' IN LN K = A + B/T FOR X < XHVD2

* SDEHY2 -7241.E0 1 'B' IN LN K = A + B/T FOR X < XHVD2

* ADEHY3 4.632E0 1 'A' IN LN K = A + B/T FOR X < XHVD3

* SDEHY3 -7546.E0 1 'B' IN LN K = A + B/T FOR X < XHVD3

* DHVY1 2.865E 1 Decomposition enthalpy 3/kg H2O: 1st step

* DHVY2 3.705E 1 Decomposition enthalpy 3/kg H2O: 2nd step

* DHVY3 3.705E 1 Decomposition enthalpy 3/kg H2O: 3rd step

* PRHY1 1.0 1 Hydride production rate law multiplier

* FCNHY 1.0 1 Hydride consumption rate law multiplier

* FNHY1 1.0 1 Nitriding rate law multiplier

* PUMP, FEED, AND CONDENSER MODELS

* SYNCRP 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

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* IRPUM 1 1 Pump inlet region

* IRPUM 1 1 Pump inlet region

```

* 1=number of fuel rods+1. If there is no insert, number of fuel
* rods+1.
*
FVUEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
0.316 0.027 0.316 0.158 0.018 0.009 0.009 0.000
0.176 0.316 0.000 0.167 0.158 0.316 0.167 0.022
0.018 0.316 0.334 0.167 0.306 0.018 0.158 0.107
0.000 0.018 0.158 0.018 0.000 0.000 0.018 0.158
0.000 0.009 0.018 0.000 0.000 0.000 0.000 0.158
0.000 0.000 0.018 0.167 0.316 0.048 0.258
0.000 0.000 0.000 0.018 0.176 0.343 0.460 0.106
*
* gap distance for micro-convection calculation
*
XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.037 0.037 0.056 0.000 0.037 0.037 0.000
0.056 0.037 0.037 0.056 0.000 0.037 0.037 0.090
0.000 0.056 0.037 0.037 0.000 0.056 0.037 0.056
0.000 0.000 0.037 0.037 0.056 0.000 0.037 0.043
0.000 0.000 0.037 0.037 0.090 0.056 0.043 0.000
END IHSTFL for 1st fuel basket
*
* 2nd Fuel Basket
*
* heat sink pairs for second fuel basket
*
IHSTFL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
IPLINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
IFLMCO 30 ! define the adjacent MCO wall heat sink
IFLID 43 ! define the lid of floor heat sink to which the fuel
! define to
APFLZ 0.131 ! flow area in the basket,
*
* fraction of geometric area exposed for oxidation
*
FAOMFL (2*33.6 m2) = 0.10417 0.10417 0.10417 0.10417 0.10417
7.0 m2 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417
FOX 10.0 0.0 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
XFLXO 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
ENHDD 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
*
* Initial amount (kg) of water per geometric surface area (m2) of fuel
*
FWFLD 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
FWFLD 0.0 ! on the outer surface of the insert
0 kg / 2.2 m2
FWFLM 0.0 ! on the inner surface of the MCO wall
0.1 ! wetted fraction of fuel surface
FWFLM 0.0 ! wetted fraction of MCO wall
FWFLM 1.0 ! wetted fraction of MCO wall
MSLEFL 1.08 ! mass of sludge particles (kg) in the fuel basket
*
* view factor matrix between the insert,

```

```

0.      ! START TIME, >0 FOR RESTART RUN
TSTART      ! RESTART FILE IS READ FROM HANSF.RER

! END TIME (Seconds)
TLAST       432000.

! MIN TIMES (Seconds)
DTMIN       0.0 0.01

! MAX TIMES (Seconds)
DTMAX       0.0 5.0

! PRINT INTERVAL (Seconds)
DTPRINT     0.0 288000.

! MIN INTERVAL WITHOUT PLOT (Seconds)
DTNPRINT    0.0 100.

! MAX INTERVAL WITHOUT PLOT (Seconds)
DTMPRINT    0.0 1000.

! FRACTIONAL CHANGE IN THERMAL MASS
DTFRST     0.0 86400.

! FRACTIONAL CHANGE IN THERMAL MASS
DTFRCH     0.005

! FRACTIONAL CHANGE FOR PLOTTING
DTFLCH     0.005

! TIMING is a comment.
PPFLCH     0.03

PLOT        ! Keyword for plotting section
Plotting syntax:

PRESSURE n rlist - Pressure, Pa
GAS-T n rlist - Gas Temperature - Inner Surface, K
GAS-F n rlist - Gas Sink Temperature - Outer Surface, K
HS-TI n rlist - Heat Sink Temperature - Average, K
HS-TO n rlist - Heat Sink Temperature - Top, K
HS-TA n rlist - Aerosol Mass ('kg/s'), kg
AKRO-M n rlist - Mass Flowrate Mass Flowrate, kg/s
GAS-WX n rlist - Counter Current Humidity
GAS-X GNSNAME n rlist - Gas Mole Fraction
GAS-RH GNSNAME n rlist - Gas Mass (Species), kg
GAS-MASS GNSNAME n rlist - Aerosol Mass (Species), kg
ASR-MASS GNSNAME n rlist - Total Mass (Species), kg
MASS GNSNAME n rlist - Deposited Mass (Species), kg
LIQ-PRESS - GASNAME n rlist - Deposition mass require a region

! Pressure, Gas Temperature, and total aerosol mass require a region
! list

* Heat Sink Temperatures need a heat sink number list

* Flowrates need a junction number list

* Gas concentration, relative humidity, individual species gas mass,
individual species aerosol mass, total (gas/aerosol), individual
species mass, and individual species deposited liquid mass require
a region and gas name
* NOTE trick here to keep plot format ALMOST the same as CVD runs
* Since no region 5, plot pressure for region 2.
*
PRESSURE 1 1 2 3 4 ! WCO Pressure
          4 1 2 3 4 ! Temp in regions 1,2,3,4 & 5
          11 31 32 33 34 35 36 37 38 39 40 41 Isocrep bucket
          HS-TI 3 42 43 44 45 46 47 48 49 50 ! Caek, Bottom and lid
          HS-TA 10 1 12 13 14 15 16 17 18 19 20 21 22 23 24 25 ! Bot. fuel
          HS-FA 5 16 17 18 19 20 21 22 23 24 25 ! Bot. fuel
          HS-TA 10 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 ! Bot. fuel
          HS-TA 10 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 ! Bot. fuel
          GAS-X NITROGEN 3 1 2 3 4 ! H2O concentration in WCO
          GAS-X OXYGEN 3 1 2 3 4 ! H2O concentration in WCO
          GAS-X STEAM 3 1 2 3 4 ! H2O concentration in WCO

```

Date: 12/31/98

B - 17

* 0 kg of water total for scrap basket; 0/7/89 = 0 kg/m³
 * initial amount (kg) of water per unit bulk volume
 * (m³) of scrap surface of the insert
 * on the outer surface of the MCO wall
 * (per unit area, m²)
 * wetted fraction of MCO wall
 * wetted fraction of surface area
 * gap distance between basket and mco wall
 * 1/4" gap for scrapbag scrap basket and mco wall
 * gap distance between particles (kg) in the scrap basket
 * mass of scrap particles
 * XSCMCO 0.06635 g distance between particles
 * HSLSC 3.1 mass of scrap particles
 * END IHSSC for lat scrap basket
 * END SCRAP_BSKT
 *
 * END MCO

B.3 MCO Staging

- MCO STAGING. HOTTEST MCO, HOTTEST SPOT 770 W, 144.6 F CSB AIR AVERAGE HYDRATE INVENTORY, BOUNDING RX AREA
- MCO INITIALLY AT 30 C INTERNALLY AFTER SHIPPING (INSENSITIVE)
- MCO WALL SURFACE COULD BE USING CSB THERMAL ANALYSIS METHODOLOGY APPLIED TO 70 W MCO
- TUBE GAP 1.5" HEIGHT 11.35 M³, AREA 25.27 M² FOR 2 MCO HAFER
- 0.144 KG HYDRATE WATER INVENTORY - BEST EST.
- 0.0 M² SCRAP, 7.0 M² TOTAL FUEL
- UNLESS OTHERWISE NOTED, MKS UNITS
- 1 TIER OF SCRAP BASKET
- 4 TIERS OF FUEL BASKETS (MODELED AS TWO FUEL BASKETS)

CONTROL : Major keyword group

* i keyword; next line is title, title can be any length
 * TITLE NVR: 108 C MCO WALL, 770 W, 0.144 KG H2O
 * COMMENT

! Keyword

FAY/98-40, Rev. 1

```

GAS-X HYDROGEN 3 1 2 3 1 H2 concentration in MCO
GAS-X HELIUM 3 1 2 3 1 H2 concentration in MCO
GAS-X 3 1 2 3 1 Uni-directional mass flowrate
GAS-W 3 1 2 3 1 Counter-current mass flowrate
GAS-WX 3 1 2 3 1 Mass of hydrogen in region 5
GAS-MASS HYDROGEN 1 1 4 1 Mass of steam in region 5
GAS-MASS STEAM 1 1 4 1 Mass of steam in region 5
END PLOT 1 PLOT is a comment
*
*
ACTIVE MODELS 1 Keyword; MODELS is a comment; 1 - on, 0 - off
*
*
JUNC 1 Junction flow model
ICCTLM 1 Counter-current flow model
INSINK 1 Heat sink
INCS 0 Concentration
INCS 0 Aerosol Sedimentation
INCS 0 Aerosol Leakage
IFOG 0 Fog formation
ISRC 0 User-defined source
INCO 1 MCO models
ISENS 0 Sensitivity runs
END ACTIVE MODELS 1 ACTIVE MODELS is a comment
*
*
C-----
C SOURCE GROUP: GROUPS REPEATED FOR INPUT # OF REGIONS
C END OF GROUP DESIGNATED BY 'REGION' OR 'END' KEYWORDS
C ENTER: TIME, TEMP, FLOWRATES, POWER
C SYNTAX EXAMPLE:
C SOURCES 2 1 --- KEYWORD AND # SOURCE GROUPS
C REGION 1 GASES 2 1 --- REGION #, # GASES
C STEAM HYDROGEN 1 --- GAS NAMES MUST BE ON NEXT LINE
C 10 300 1.E-3 1.E-3 0.E0
C 10 300 1.E-3 1.E-3 0.E0
C END REGION 1 --- ENDS A REGION SOURCE
C 1 --- FOR AEROSOL, SENSITIVITY -IVE REGION
C 1 --- ENDS ALL SOURCE INPUT
C END SOURCE
C
C END CONTROL 1 End of CONTROL keyword group
*
*
VOLUMES 4 1 total number of control volumes
*
* total MCO gas volume is 0.50 m^3
*
* Units:
* VOLUME m^3, SED_AREA m^2, ELEVATION m, TEMP_GAS K, PRESSURE Pa
* MCO top MCO middle MCO bottom environment
* 1 2 3 4
REGIONS
VOLUME 0.100 0.200 0.200 1.E9
SED_AREA 0.172 0.172 0.172 0.0
ELEVATION 2.65 1.33 0.0 0.0
TEMP_GAS 30.0 30.0 30.0 30.0
PRESSURE 1.013E5 1.013E5 1.013E5 1.013E5
END REGIONS 1 REGIONS is a comment

```

```

*
* Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
*
*
GASES 1 2 3 4
HELIUM 0.999 0.999 0.999 0.0
STEAM 0.001 0.001 0.001 0.0
OXYGEN 0.0 0.0 0.0 0.75
NITROGEN 0.0 0.0 0.0 0.0
END GASES 1 GASES is a comment
*
* Aerosol concentration of each region (kg/m^3)
* No more than five columns at a time
*
*
AEROSOLS 1 2 3 4 5
STEAM 0.0001 0.0 0.0 0.0 0.0
END AEROSOLS 1 AEROSOLS is a comment
*
* No more than five columns at a time, so continue with 6 & 7
*
*
AEROSOLS 6 7
STEAM 0.0 0.0
END AEROSOLS 1 AEROSOLS is a comment
*
* OPTIONAL TEMPERATURE AND PRESSURE CONTROL
* CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
* IMPOSE TEMPERATURE LOOK-UP TABLE
* SYNTAX:
* OFFSET TIMEGTG
* EXTRAPOLATION TIMEGTG
* TIMEGTG IREG TIME1, TIME2...TIMELAST
* TGTG IREG TIME1, TIME2...TEMPLAST
* LINEAR INTERPOLATION BETWEEN VALUES
*
* SIMILAR SYNTAX FOR PRESSURE:
* OFFSET TIMEGTG
* EXTRAPOLATION TIMEPG
* TIMEPG IREG PRES1, PRES2...PRESSURES ARE IN PA!!
* PREFIX IREG PRES1, PRES2...PRESSURES ARE IN PA!!
*
* OFFSET TIMEGTG= TIME-OFFSET TIMEGTG
* EXTRAPOLATION TIMEGTG= LAST TO USE LAST VALUE IN THE TABLE,
* - EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
* - PERIOD TO WRAP AROUND.
*
*
OFFSET TIMEGTG 0.0
EXTRAPOLATION TIMEGTG LAST
TIMEGTG 4 0.0 1.E5 10.E5
TGTG 4 10E.0 10E.0 10E.0
*
* CONTROL MCO BOUNDARY P, 30.
* OFFSET TIMEGTG
* EXTRAPOLATION TIMEGTG EXTRAP
* TIMEGTG 1 0.0 100.
* PREFIX 1 1.E5 1.2E5 1.4E5
*

```

B - 19

* TMS	0.0
TREGO	4
TOHS	0.0
XLHS	3.95
EHSI	0.3
EHSO	0.3
END	*
DUMMY	PUP LIDS NT 108 C
TUBE WALL	MCO BOT
42	43
* SINKS	1
IGROM	8000.
RHO	16.0
CRRH	500.0
QV	0.0
XRI	0.3199
XRO	0.045
AHS	0.29
TUNIT	108.00
TOINIT	108.00
IMSLAB	10
IIRGI	3
TIRS	1
TREGO	0.0
TOHS	0.0
XLHS	3.950
EHSI	0.25
EHSO	0.25
END	*

† TEMPERATURE

```

* * * * *
* SYNTAX:
*
* OFFSET_TIMEHS
*
* * * * *
* EXTRAPOLATION TIMEHS
*
* * * * *
* TIMINHS IHS ISD TIME1, TIME2...
*
* * * * *
* MAXIHS IHS ISD TEMPI, TEMP2..
*
* * * * *

```

* IHS = HEAT SINK NO.; ISD = SIDE NO. (1 OR 2) FOR IHS

* CONTROL HEAT SINK BOUNDARY 1

★	OFFSET_TIMES	U. EXTRAP
1	0.000000	0.000000
2	0.000000	0.000000
3	0.000000	0.000000
4	0.000000	0.000000
5	0.000000	0.000000
6	0.000000	0.000000
7	0.000000	0.000000
8	0.000000	0.000000
9	0.000000	0.000000
10	0.000000	0.000000
11	0.000000	0.000000
12	0.000000	0.000000
13	0.000000	0.000000
14	0.000000	0.000000
15	0.000000	0.000000
16	0.000000	0.000000
17	0.000000	0.000000
18	0.000000	0.000000
19	0.000000	0.000000
20	0.000000	0.000000
21	0.000000	0.000000
22	0.000000	0.000000
23	0.000000	0.000000
24	0.000000	0.000000
25	0.000000	0.000000
26	0.000000	0.000000
27	0.000000	0.000000
28	0.000000	0.000000
29	0.000000	0.000000
30	0.000000	0.000000
31	0.000000	0.000000
32	0.000000	0.000000
33	0.000000	0.000000
34	0.000000	0.000000
35	0.000000	0.000000
36	0.000000	0.000000
37	0.000000	0.000000
38	0.000000	0.000000
39	0.000000	0.000000
40	0.000000	0.000000
41	0.000000	0.000000
 
87	0.000000	0.000000
88	0.000000	0.000000
89	0.000000	0.000000
90	0.000000	0.000000
91	0.000000	0.000000
92	0.000000	0.000000
93	0.000000	0.000000
94	0.000000	0.000000
95	0	

* EXTRAPOLATION TIMES

TIME	SH	TH	15	2	0.0	1.86	1.00	0
1.86	1.00	0						

THSFX	15	2	108.0	108.0
THSFX	15	2	108.0	108.0

1.56
TIMTHS 30 2 0.0

THSFIX	30	2	108.0	108.0
11111111				

INSTRUMENT	TIME	WAVELENGTH	WAVELENGTH	WAVELENGTH
41	2	0.0	1.0	1.0
41	2	0.0	1.0	1.0
41	2	0.0	1.0	1.0

THSETX	41	2	108.0	108.0
TIMING	41	2	108.0	108.0

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 IT IS NOT A COPY OF THE ORIGINAL DOCUMENT

* * *

* ETV CASK AND ENVIRONMENT; MCO SHOULD FOLLOW

* FIX CASK AND ENVIRONMENT; NOT ENGINEER

1.E6

* TIMTHS 42 1	0.0	1.00
-----	1.00 0	108.0

THSFX	42	1	108.0	108.0
*				1.E6

* TIMTHS	42	2	0.0	1.00
				108 0

★	THSFX	42	2	108.0	108.0
★	THSFX	42	2	108.0	108.0

→

→

END HEAT SINKS ! HEAT_SINKS is a comment

END HEAT STAMP. 11-11-66

★ ----- JUNCTIONS 3 ! 3 Junctions

JUNCTIONS 3 1 3 CONJUNCTIONS

FBI/DOJ Rev. 1-1-80

1/11/98-10, N.Y. I

Date: 12/31/98

```

FAOXFL 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417
FOX 10.0 0.0 ! multiplier for FAOXFL
FXLOX0 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
FXHVD0 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
* initial amount (kg) of water per geometric surface area (m2) of fuel
* kg / (2*33.6 m2)
FWFL0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
FWFL10 0.0 ! on the outer surface of the insert
FWFLM0 0.0 ! on the inner surface of the MCO wall
FAWFL 0.1 ! wetted fraction of fuel surface
FAWFLM 1.0 ! wetted fraction of MCO wall
MSLFL 1.08 ! mass of sludge particles (kg) in the fuel basket
* view factor matrix between the insert,
* and the MCO wall. Therefore, the dimension of the square matrix is
* #number of fuel rods+1. If there is no insert, number of fuel
* rods+1.
FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
0.316 0.027 0.316 0.157 0.000 0.000 0.000 0.000
0.176 0.157 0.316 0.158 0.000 0.000 0.009 0.000
0.009 0.316 0.334 0.167 0.316 0.316 0.167 0.022
0.000 0.018 0.158 0.158 0.000 0.018 0.018 0.107
0.000 0.009 0.000 0.158 0.018 0.018 0.158 0.208
0.000 0.000 0.018 0.167 0.316 0.316 0.167 0.022
0.000 0.000 0.000 0.018 0.167 0.316 0.316 0.460 0.106
* gap distance for micro-convection calculation
XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.037 0.037 0.037 0.056 0.056 0.000 0.000
0.037 0.037 0.000 0.037 0.037 0.037 0.037 0.000
0.056 0.037 0.037 0.037 0.000 0.037 0.037 0.000
0.000 0.056 0.037 0.037 0.037 0.000 0.056 0.037 0.056
0.000 0.056 0.000 0.037 0.037 0.037 0.056 0.000
0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.000
0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.000
END IHSEFL for 1st fuel basket
END IHSEFL for 2nd fuel basket
*
* SCRAP_BSNT 1 ! Total number of scrap baskets
*
IHSSC 31 ! ring 1, theta
32 33 ! ring 2, theta
34 35 ! ring 3 & 4, radial
37 36 ! ring 6 & 5, radial
38 39 ! ring 11 & 12, radial
*
ISCSINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
ISCSFIN 40 ! define copper fin heat sink

```

```

FAOXFL 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417 0.10417
FOX 10.0 ! multiplier for FAOXFL
FXLOX0 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
FXHVD0 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5
1.0 1.0 1.0 1.0 1.0 1.0 1.0
* initial amount (kg) of water per geometric surface area (m2) of fuel
* kg / (2*33.6 m2)
FWFL0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
FWFL10 0.0 ! on the outer surface of the insert
FWFLM0 0.0 ! on the inner surface of the MCO wall
FAWFL 0.1 ! wetted fraction of fuel surface
FAWFLM 1.0 ! wetted fraction of MCO wall
MSLFL 1.08 ! mass of sludge particles (kg) in the fuel basket
* view factor matrix between the insert,
* and the MCO wall. Therefore, the dimension of the square matrix is
* #number of fuel rods+1. If there is no insert, number of fuel
* rods+1.
FVIEW 0.492 0.316 0.176 0.009 0.000 0.000 0.000 0.000
0.316 0.027 0.316 0.157 0.000 0.000 0.000 0.000
0.176 0.157 0.316 0.158 0.000 0.000 0.009 0.000
0.009 0.316 0.334 0.167 0.316 0.316 0.167 0.022
0.000 0.018 0.158 0.158 0.000 0.018 0.018 0.107
0.000 0.009 0.000 0.158 0.018 0.018 0.158 0.208
0.000 0.000 0.018 0.167 0.316 0.316 0.167 0.022
0.000 0.000 0.000 0.018 0.167 0.316 0.316 0.460 0.106
* gap distance for micro-convection calculation
XGAP 0.000 0.037 0.037 0.056 0.000 0.000 0.000 0.000
0.037 0.037 0.037 0.037 0.056 0.056 0.000 0.000
0.037 0.037 0.000 0.037 0.037 0.037 0.037 0.000
0.056 0.037 0.037 0.037 0.000 0.037 0.037 0.000
0.000 0.056 0.037 0.037 0.037 0.000 0.056 0.037 0.056
0.000 0.056 0.000 0.037 0.037 0.037 0.056 0.000
0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.000
0.000 0.000 0.000 0.037 0.037 0.037 0.056 0.000
END IHSEFL for 1st fuel basket
END IHSEFL for 2nd fuel basket
*
* 2nd Fuel Basket
*
heat sink pairs for second fuel basket
IHSEFL 16 17 18 19 20 21 22 23 24 25 26 27 28 29
IIFLINS 0 ! define the adjacent center insert heat sink,
! 0 for no insert
IIFLMCO 30 ! define the adjacent MCO wall heat sink
IIFLID 43 ! define the lid or floor heat sink to which the fuel
! radiate to
AFLFL 0.131 ! flow area in the basket,
* fraction of geometric area exposed for oxidation
* 7.0 m2 / (2*33.6 m2) = 0.10417

```

B-23

FAT/98 40, Rev. 1

	* porosity of the scrap for each heat sink in the order read in	
ISCONCO 41	! define the adjacent MCO wall heat sink	
ISCNCD 44	! define the lid or floor heat sink to which the scrap	
	! radiate to	
*	* porosity of the scrap for each heat sink in the order read in	
(* (31, 32, 33, 34, ...)	, 0.45 0.45 0.45 0.73 0.73 0.73 0.73	
PFOROS 0.45	size for each scrap heat sink in the order read in (m)	
characteristics	0.0635 0.0635 0.0635 0.0635 0.0635 0.0635	
XDCSCRIP	0.0254 0.0254 0.0254 0.0254	
XSCBCK	radius of scrap basket (m)	
XHSCBK	height of scrap basket (m)	
XHSBCBK 0.691	! height of scrap basket for oxidation	
*	* exposed surface area available for oxidation	
	* per unit volume of scrap (l/m) for	
	* each scrap basket heat sink in the order read in	
	* Example: bounding oxidation area: 6/0.17491 = 34.30 l/M	
(*	m ² / 0.17491 = 9.71	
XNOXSC 34.3	34.3 34.3 34.3 34.3 34.3 34.3	
FONKSC	10.0 0.0 ! multiplier FOR AVOXSZ	
XSCOXO 4.0e-5	4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5 4.0e-5	
FSCHVD 1.0	1.0 1.0 1.0 1.0 1.0 1.0	
WVSVCDO 0.0	total for scrap basket; 0/0.17491 = 0 kg/m ³	
FWNSCZO 0.0	initial mass of scrap	
FWNSCZO 0.0	! on the outer surface of the insert	
FWNSCZO 0.0	! (per unit area, m ²)	
FWNSCZO 0.0	! on the inner surface of the MCO wall	
FWNSCZO 0.0	! (per unit area, m ² surface area	
FANMSC 0.1	! wetted fraction of MCO wall	
FANMSC 1.0	! wetted trace between the insert and scrap basket	
XSCINS 0.01	! gap depth for scrap basket and mco wall	
XSCMCO 0.0	! gap distance between scrap basket and MCO wall	
HSLSCS	! mass of sludge particles (kg) in the scrap basket	
END SCRAP_BSKT		
END MCO		

3.1.1.1. Driving With Axial Variation in Fuel Damage

```

* CASE VCIAMF: INDEFINITE VACUUM CYCLE,
* ONE SCRAP BASKET AT THE TOP (FFFFF)
*
*
* REACTION AREA = 4.5 M*2 PER SCRAP BASKET
* 0.875 M*2 PER FUEL BASKET
*
*
* the run
*
* 0.01
* 0.
* 100.
* 500.
* 2.0
*
* will cause the code to use minimum time step of 0.0
* for the first 100 seconds, 1.0 second for next 400
* seconds, and then 2.0 second for the rest of
* the run

```

Date: 3/05/99

B-24

FBI/98-40, Rev. 2

Date: 3/05/99

B-24

FBI/98-40, Rev. 2


```

END CONTROL      ! End of CONTROL keyword group
*
*-----
* VOLUMES      7      ! total number of control volumes
*-----
* total MCO GAS volume is 0.55 m^3, 0.55/3=0.183 per each node
* No more than 5 columns (regions) at a time
* Units:
* VOLUME m^3, SED AREA m^2, ELEVATION m, TEMP GAS C, PRESSURE Pa
*-----
Regions 1 to 5 each contain a basket, top to bottom
scrapi fuel1 fuel2 fuel3 fuel4 fuel5
*-----
REGIONS
VOLUME      0.100      0.100      0.100      0.1
SED AREA    0.172      0.172      0.172      0.172
ELEVATION   2.65       2.00       1.32      0.66      0.0
TEMP GAS    50.0       50.0       50.0       50.0
PRESSURE    1.013E5    1.013E5    1.013E5    1.013E5
END REGIONS
*
gap environment
REGIONS
SED AREA    0.25       1.89
ELEVATION   0.0        0.0
TEMP GAS    50.0       50.0
PRESSURE    1.013E5    1.013E5
END REGIONS ! REGIONS is a comment
*
Gas composition of each region; specify mole fraction of each gas
* No more than five columns at a time
*-----
GASES
HELIUM      1      2      3      4      5
HELIUM      0.89     0.89     0.89     0.89     0.89
STEAM       0.11     0.11     0.11     0.11     0.11
OXYGEN       0.0      0.0      0.0      0.0      0.0
NITROGEN     0.0      0.0      0.0      0.0      0.0
WATER        0.0      0.0      0.0      0.0      0.0
END GASES
*
* If there are more than five regions, continue here.
*-----
GASES
HELIUM      6      7
HELIUM      0.0      0.0
STEAM       0.0      0.0
OXYGEN       0.0     0.21
NITROGEN     0.0     0.79
WATER        1.0
END GASES
! GASES is a comment
*
Aerosol concentration of each region (kg/m^3)
* No more than five columns at a time
*-----
AEROSOLS
STEAM       1.0001    2      3      4      5
AEROSOLS    0.0001    0.0      0.0      0.0      0.0
END AEROSOLS ! AEROSOLS is a comment
*
No more than five columns at a time, so continue with 6 & 7
*-----
AEROSOLS      6      7
AEROSOLS     0.0      0.0
END AEROSOLS ! AEROSOLS is a comment
*
OPTIONAL TEMPERATURE AND PRESSURE CONTROL
CONTROL MCO HEATUP GASES AND MCO INLET GAS TEMPERATURE
IMPOSE TEMPERATURE LOOK-UP TABLE
SYNTAX:
OFFSET_TIMETG
EXTRAPOLATION_TIMETG
TGFX IREG TIME1, TIME2...TIMELAST
TGFI IREG TIME1, TIME2...TIMELAST
TEMPERATURES ARE IN K!!!
LINEAR INTERPOLATION BETWEEN VALUES
SIMILAR SYNTAX FOR PRESSURE:
EXTRAPOLATION_TIMETG
OFFSET_TIMETG
TIME IREG TIME1, TIME2...TIMELAST
TGFI IREG PRES1, PRES2...PRESSURES ARE IN PA!!!
OFFSET_TIMETG- OFFSET TIME: ENTER LOOKUP TABLE WITH
TIME+OFFSET TIMETG
EXTRAPOLATION_TIMETG- LAST TO USE LAST VALUE IN THE TABLE,
= EXTRAP TO EXTRAPOLATE FROM LAST TWO POINTS,
= PERIOD TO WRAP AROUND.
*
OFFSET_TIMETG 50.
EXTRAPOLATION_TIMETG LAST
TIME1 1 0.0 100. 200.
TGFI 1 20.0 100. 200.
CONTROL MCO BOUNDARY P, 30.
OFFSET TIMETG
EXTRAPOLATION TIMETG EXTRAP
TIME 1 0.0 100. 200.
PREFIX 1 1.E5 1.2E5 1.4E5
END VOLUMES ! VOLUMES is a comment
*
Major keyword-----
HEAT SINKS      84      ! Total number of heat sinks
*-----
* No more than 5 columns at a time,
* Repeat the following structure,
* SINKS
*-----
* END
*
Syntax:
! for plane, 0 or 2 for cylinder
! GEOM
! material type
! INHTS
! KHS
! Thermal Conductivity (W/m/K), if different from material type
! CHPS
! Specific Heat (J/kg/K), if different from material type
! QV
! Volumetric Heat Generation (W/m^3), if different from material type

```

Date: 3/05/99

END	*	21	22	23	24	25
SINKS						
IGSOM	0	0	0	0	0	
IRKHS	1	1	1	1	1	
XRI	0.02160	0.00610	0.02160	0.00610	0.02160	
XRO	0.03075	0.01625	0.03075	0.01625	0.03075	
ANS	0.655	0.557	1.310	0.278	0.655	
XHS	0.663	0.661	0.663	0.661	0.663	
TUNIT	50.00	50.00	50.00	50.00	50.00	
TOINIT	50.00	50.00	50.00	50.00	50.00	
INSLAB	3	3	3	3	3	
IREGI	4	4	4	4	4	
THS	0.0	0.0	0.0	0.0	0.0	
IREGO	4	4	4	4	4	
TOHS	0.0	0.0	0.0	0.0	0.0	
XLHS	0.663	0.661	0.663	0.661	0.663	
END						MO

	6	7	8	9	10
END *					
* SINKS					
* IGEOM	0	0	0	0	0
* IMATHS	1	1	1	1	1
XRI	0.02160	0.00610	0.02160	0.00610	0.02160
XRO	0.03075	0.01625	0.03075	0.01625	0.03075
MRS	0.6955	0.357	1.310	0.66	0.695
RZHS	0.663	0.340	1.310	0.66	0.663
TINAT	50.00	50.00	50.00	50.00	50.00
TONTIT	50.00	50.00	50.00	50.00	50.00
IMSIAE	3	3	3	3	3
IRSGI	3	3	3	3	3
TIHS	0.0	0.0	0.0	0.0	0.0
TRGO	3	3	3	3	3
IRGO	0	0	0	0	0

SINKS	26	27	28	29	30																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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B - 29

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*
* MATERIAL LIBRARY
* MATERIAL LIBRARY - SPECIFY MATERIAL PROPERTIES FOR MATERIAL 'imathe'
* UPTO 20 (IMAT) MATERIALS CAN BE SPECIFIED
* SYNTAX:
*   name      imathe  rho  khs  cp  qv  ehsl
* URANIUM     1      17102. 26.9 130. 1957. 0.7
* 0.7
* 0. STAINLESS-STEEL 2 8000. 16.0 500. 0. 0.3
* 0. COPPER      3      8954. 398.0 384. 0. 0.7
* 0.7
* END
*
* SANDWICH HEAT SINKS - STRING TOGETHER NUMER OF CONSECUTIVE HEAT SINKS
* TO MIMIC A SANDWICH WALL. UPTO 100 SANDWICH WALLS CAN BE SPECIFIED,
* WITH 0 TO 10 LAYERS IN EACH WALL. THE SANDWICH HEAT SINK SERIES SHOULD BE
* ARRANGED SUCH THAT THE OUTER FACE OF THE FIRST HEAT SINK AND THE
* INNER FACE
* OF THE LAST HEAT SINK IN THE SERIES FACE THE GAS REGIONS (OR
* INSULATED).
* SYNTAX:
* SANDWICH hsl hsep1 ha2 hsep2 ha3 hsep3 ... han
* hsl is the gap conductance (W/m^2/C) between the layers
* hsep1 to hsep3 are the gap conductance (W/m^2/C) between the layers
* BETWEEN THE INSERT AND THE DIP TUBE, THERE IS A AIR GAP OF THICKNESS
* 0.00076 M. THEREFORE, THE GAP CONDUCTANCE IS 0.03/0.00076=40 W/m^2/C
* SANDWICH 75 40. 76
* SANDWICH 77 40. 78
* SANDWICH 79 40. 80
* SANDWICH 81 40. 82
* SANDWICH 83 40. 84
*
* Represent the thermal resistance in the spokes in the scrap basket
* 12 spokes, 1/8"(0.003175m) thick, 0.676 m high, and 0.191 m long
* Therefore, the gap conductance is:
* 398/0.191*(12*0.003175/(2*3.14*0.2842))=44.48 W/m^2/C
* SANDWICH 62 44.48 63
* SANDWICH 496 44.48 497
* SANDWICH 509 44.48 510
* SANDWICH 522 44.48 523
*
* TEMPERATURE DEPENDENT EMISSIVITY:
* USER CAN INPUT A TEMPERATURE DEPENDENT EMISSIVITY BY INPUTTING A
* NEGATIVE INTEGER FOR THE EMISSIVITY AND PROVIDING THE CORRESPONDING
* TEMPERATURE VERSUS EMISSIVITY LOOK-UP TABLE.
* SYNTAX:
* TABLE n temperature-entry(C)
* TABLE n emissivity-entry
* designator n is the table
*
* TEMPERATURE DEPENDENT EMISSIVITY:
* USER CAN DEFINE CONDUCTION NETWORKS
* SYNTAX:
* COND_NETWORK ihsl iha2 ihs3 .... ihsn upto 100 heat
* sinks

```

```

*
* COND_NETWORK ihsl iha2 ihs3 .... ihsn upto 100 heat
* sinks
*
*
* upto 5 networks
*
* MUST BE ORDERED TOP TO BOTTOM TO BE CONSISTENT WITH AXIAL
* MODALIZATION. GIVIOUS DIP TUBE CONNECTED TO THE SHIELD PLUG(HS #74)
* COND_NETWORK 74 84 82 76 78 80
* MODEL CONTIGUOUS INSERT CONNECTED TO THE SHIELD PLUG(HS #74)
* COND_NETWORK 74 83 81 75 77 79
* MODEL CONTIGUOUS MCO WALL CONNECTED TO THE SHIELD PLUG(HS #74)
* COND_NETWORK 74 71 60 15 30 45
*
* USER CAN CONTROL HEAT SINK BOUNDARY TEMPERATURE
* SYNTAX:
* OFFSET TIMERS
* EXTRAPOLATION TIMERS
* TIMHS IHS ISD TIMP1, TIME2...
* TIMHS IHS ISD TIMP1, TIME2...
* IHS = HEAT SINK NO.; ISD = SIDE NO. (1 OR 2) FOR IHS
* CONTROL HEAT SINK BOUNDARY T
* EXTRAPOLATION TIMERS 0 EXTRAP
* TIMHS 15 2 0.0 1.56
* TIMHS 15 2 50.0 50.0
* TIMHS 30 2 0.0 1.56
* TIMHS 30 2 50.0 50.0
* TIMHS 45 2 0.0 1.56
* TIMHS 45 2 50.0 50.0
* TIMHS 60 2 0.0 1.56
* TIMHS 60 2 50.0 50.0
* TIMHS 71 2 0.0 1.56
* TIMHS 71 2 50.0 50.0
* TIMHS 72 1 0.0 1.56
* TIMHS 72 1 50.0 50.0
* TIMHS 72 2 0.0 1.56
* TIMHS 72 2 50.0 50.0
* TIMHS 73 2 0.0 1.56
* TIMHS 73 2 50.0 50.0
*
* END HEAT SINKS ! HEAT_SINKS is a comment
*
* JUNCTIONS 5 ! # of Junctions
*
* 1) MCO fuel 4 to fuel 3 5->4
* 2) MCO fuel 2 to fuel 1 4->3
* 3) MCO fuel 1 to scrap 1 3->2
* 4) MCO fuel 1 to scrap 1 2->1
* 5) MCO top to Outlet volume, 1->7 (deactivated)
*
* Syntax:
* 1) JTYTP
* 2) JTYTP
* 3) JTYTP
* 4) JTYTP
* 5) JTYTP
*
* Junction Type: 1 = Normal, 2 = HEPA, 3 = Cover, 4 = Failure,
* 5 = Check valve
* for failure junction, it is the pressure differential
* required

```

rate

* to fall from the upstream compartment to the downstream

* compt. for check valve junction, it is the differential pressure

* required to open the junction from upstream to downstream

* only. for failure junction, it is the pressure differential

* required to fall from the downstream compartment to the upstream

* compt. for check valve junction, it is the differential pressure

* at which the opened check valve closes

* IFAN Fan type: 1 = constant volumetric flow fan

* WFFAN volumetric flow rate of the fan, for constant dolt P fan,

* the volumetric flow rate is converted to the corresponding

* Upstream Region

* IR1 Downstream Region

* IR2 Area (m²)

* AJN Bypass area for HEPA junction (m²)

* PHEPA HEPA Filter Failure Pressure (Pa)

* ACOV Cover Area (m²)

* MCOV Cover Height (m)

* Z1N Elevation at floor of IR1

* Z2N Elevation at floor of IR2

* C2N Loss coefficient multiplies 0.5*rho*v²

* XHZN Orientation: 1 = horizontal, 0 = vertical

* IHORIZ Characteristic width, m

* XHJN Characteristic height, m

* XLJN Characteristic length, m

* DFJN Decontamination Factor

* N90 No. of 90 bends

* PATHS 1 2 3 4 5

* IJTV 1 1 1 1 1

* IR1 5 4 3 2 7

* IR2 4 3 1 1 1

* IHORIZ 1 0.61 0.61 0.61 2.54E-2

* XHJN 0.61 0.61 0.61 2.54E-2

* XLJN 0.91 0.01 0.01 10.

* AJN 0.025 0.025 0.025 0.0078 0.0

* Z1N 1.2 1.2 1.2 1.2 10.

* Z2N 0.0 0.0 0.0 0.0 12.65

* C2N 1.0 1.0 1.0 1.0 4.0

* DFJN 1.0 1.0 1.0 1.0 1.0

* N90 0 0 0 0 3

* END PATHS 1 PATHS is a comment.

* END JUNCTIONS 1 JUNCTIONS is a comment.

* MCO 1 MCO Major Keyword

* GENERAL 1 Keyword for general inputs

* IOMD 2 1 = 0, disable oxidation of fuel/scraper

* 1 = 1, do oxidation of fuel/scraper

* 1 = 2, oxidation of covered surface uses water prop for

! =1, do hydrating/dehydrating calculation

! =0, disable hydrating/dehydrating calculation

! =1, initial heat transfer calculation

! =0, normal diversion heat transfer calculation

! =2, suppress the individual diversion when QDVRT>0 but TFI-Tgas, or QDVRT<0 but TFI-Tgas

! =3, suppress the individual diversion when QDVRT>0 but TFI-Tgas

! =1, do evaporation/condensation of water

! =0, disable evaporation/condensation

! =1, oxidation rate law, 1 = McGillivray/Ritchie 2 = Trimble

! =1, de-entrainment of aerosol due to scrap basket

! =0, disable de-entrainment calculation

! =1, do entrainment of sludge particle calculation

! =0, disable entrainment calculation

! =0, do decomposition of fuel oxide hydrate

! =0, disable hydrate decomposition calculation

! =1, do nitrating calculation

! =0, disable nitrating calculation

! =1, do radiolysis calculation

! =0, disable radiolysis calculation

! =0, normal depletion of hydride (rate decreases with mass)

! =1, use constant hydride reaction area corresponding to the initial hydride inventory

! =2, use constant reaction area but the area goes to zero when all the mass is depleted

! =1, the fraction of the oxygen reacting with uranium hydride, which produces hydrogen instead of water

* XDHVD 2.E-5 average diameter of hydride particle (m). this is overridden by basket specific parameters, MDHYFL & XDHVSC

! =72 define the cask heat sink

! =6 define the gap node (between MCO wall and the cask)

! =1, radiative/convective h.t. between the MCO wall and the cask is computed and some of the heat is diverted to gas for stability

XGPCSK 0.0155 gap distance between the MCO wall and the cask

PHMLID 1.0 =0, turn off the radiative heat transfer between the fuel/scraper and the lid/floor

RHOSEL 5000. =1, fully account for the radiative heat transfer

SASL 1000. sludge particle density (kg/m³)

XDML 1.E-6 sludge specific area (m²/m³)

* Hydrate Model: two-step decomposition,

* input curves for in P and in K

* first step for x > XHVD2, second step for x < XHVD2

* From Technical Databook Rev. 6, page 11,

* sludge mass in two scrap baskets = 0.9 + 15.6 = 16.5 kg.

* Therefore, each scrap basket has 8.25 kg of sludge.

```

* ICONPM - Node to which the condensed steam is dumped for book-keeping
* ITFED - If non-zero, overrides TGFED with the designated region
* temperature. Used to specify time-varying feed temperature
* WVPUM - Pump volumetric flowrate (m3/s)
* WVPUM - Pump volumetric flowrate (m3/s)
* WVPUM - Feed temperature (C)
* WVPUM - Condenser cooling coil temperature (C)
* TCONPM - Condenser cooling coil temperature (C)
* 35 FT3/MIN * 1 MIN/60 SEC * 0.02832 M3/1 FT3 = 0.01652 M3/SEC
* PUMP IRIPUM ICONPM ITFED WVPUM WVPED TGFED TCONPM
* PUMP 1 7 0 0 1.652E-2 0.0 0.0 0.0
*
* Radiolysis parameters
*
* FRAD 1.0 ! multiplier for radiolysis
* FALPHA 0.197 ! alpha fractional heat load
* FBETA 0.486 ! beta fractional heat load
* FGAMMA 0.317 ! gamma fractional heat load
* OPHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
* OPHOTO 2.4E-6 ! heat deposition rate in MCO free water per gram
* GENERAL ! GENERAL is a comment
* END GENERAL
*
* PLOT ! Keyword for MCO-specific plotting section
* ! A plot file with the name 'input deck name'. PL1 is
* generated
*
* Plotting syntax:
* PUMP#2 - Hydrogen flow rate into the vacuum pump, kg/s
* OHS-H2O n list - Hydrogen flow rate through junctions, kg/s
* HS-H2O n list - Hydrogen generation rate by fuel/scraper corrosion
* WH2F1 n list - Water mass on heat sink surfaces, kg
* WH2F2 n list - Water mass on sludge on heat sink surfaces, kg
* WH2F1 n list - Hydrogen generation rate by corrosion/dehydrating/
* radiolysis in fuel baskets, kg/s
* WH2F2 n list - total hydrogen generation by corrosion/dehydrating/
* radiolysis in MCO, kg/s
* WH2TF - cumulative hydrogen generated in MCO, kg
*
* ODECF1 n list - decay heat in fuel baskets, W
* ODECS n list - decay heat in scrap baskets, W
* ODECT n list - total decay heat in MCO, W
* UDECT - cumulative decay heat in MCO, J
*
* QOXF1, QOXSC, QOXOFT, UOXOFT - fuel corrosion by O2 heat
* QOXF1, QOXSC, QOXOFT, UOXOFT - fuel corrosion by H2O heat
* QOXF1, QOXSC, QOXOFT, UOXOFT - nitriding heat
* QOXF1, QOXSC, QOXOFT, UOXOFT - dehydrating/dehydrating heat
* QOXF1, QOXSC, QOXOFT, UOXOFT - total energy in
*
* QOXF1, QOXSC, QOXOFT, UOXOFT - heat loss to MCO wall
* QOXF1, QOXSC, QOXOFT, UOXOFT - heat loss to lid/floor/insert
* QOXF1, QOXSC, QOXOFT, UOXOFT - heat loss to gas
* QOXF1, QOXSC, QOXOFT, UOXOFT - heat loss due to evaporation
* QOXF1, QOXSC, QOXOFT, UOXOFT - heat loss by axial conduction
* QOXF1, QOXSC, QOXOFT, UOXOFT - total energy out
*
* UOXOFT - total energy in fuel
* UOXOFT - initial energy in fuel + integrated(source-sink)
* UOXOFT

```

```

* Sludge mass in three fuel baskets = 0.24 + 3.24 = 3.48 kg.
* Therefore, each fuel basket has 1.16 kg of sludge.
*
* From the same Databook, page 28, the sludge water content in one
* basket and four fuel basket is given as 0.777 kg, and in two scrap
* basket and three fuel basket is given as 1.189 kg. Solving for
* sludge content in each scrap and fuel basket yields 0.073 kg per fuel
* basket
* and 0.485 kg per scrap basket.
*
* Since the uranium oxide hydrate is made of two moles of water for
* each
* mole of UO3, the fraction of sludge that is hydrated is given by
* solving equation:
* scrap - 0.485 = 36/322 * fhyd1 + 8.25, or fhyd1=0.526
* fuel - 0.073 = 36/322 * fhyd1 + 1.16, or fhyd1=0.563
* Thus, there is a slight inconsistency depending on whether we use
* scrap
* sludge data or fuel sludge data. We will use fhyd1=0.535.
*
* FHYSL 0.535 ! fraction of sludge that is hydrated
* FHYSL 2.0 ! stoichiometry number of hydrate: no. of moles of
* water per mole of uranium oxide (UO3.H2O)
*
* XHYD2 1.0 ! H2O/U ratio (stoich. number) to switch
* XHYD3 0.5 ! from first to second correlation
* ! from second to third correlation
*
* 'A' IN LN P = A + B/T FOR X > XHYD2
* 'B' IN LN P = A + B/T FOR X > XHYD2
* 'A' IN LN P = A + B/T FOR X < XHYD2
* 'B' IN LN P = A + B/T FOR X < XHYD2
* 'A' IN LN P = A + B/T FOR X < XHYD3
* 'B' IN LN P = A + B/T FOR X < XHYD3
*
* 'A' IN LN K = A + B/T FOR X > XHYD2
* 'B' IN LN K = A + B/T FOR X > XHYD2
* 'A' IN LN K = A + B/T FOR X < XHYD2
* 'B' IN LN K = A + B/T FOR X < XHYD2
* 'A' IN LN K = A + B/T FOR X < XHYD3
* 'B' IN LN K = A + B/T FOR X < XHYD3
*
* DHHY1 2.793E0 ! Decomposition enthalpy J/kg H2O: 1st step
* DHHY1 -5111.E0 ! Decomposition enthalpy J/kg H2O: 2nd step
* DHHY2 6.348E0 ! Decomposition enthalpy J/kg H2O: 3rd step
* DHHY2 -7241.E0 ! hydride production rate law multiplier
* FPROH 1.0 ! hydride consumption rate law multiplier
* FCONH 1.0 ! nitriding rate law multiplier
* FNTRI 1.0 ! nitriding rate law multiplier
*
* PUMP, FEED, AND CONDENSER MODELS
*
* SYNCR:
* PUMP IRIPUM IRIPUM ICONPM ITFED WVPUM WVPED TGFED TCONPM
*
* Definitions:
* IRIPUM - Pump inlet region
* IROPUM - Pump outlet region

```

B - 33

FAI/98-40, Rev. 2

```

* define the heat sinks comprising the first fuel basket (must be
  in pairs, for inner and outer elements)
  IHSEL 1 2 3 4 5 6 7 8 9 10 11 12 13 14
*
* IFLINS 75 ! define the adjacent center insert heat sink,
* IFLMCO 15 ! define the adjacent MCO wall heat sink
*
* initial amount (kg) of water per geometric surface area (m2) of fuel
  * 6 kg / (16.8 m2) = 0.3571
  FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
  FWEL0 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571 0.3571
  END IHSEL for 2nd fuel basket
*
* 3rd Fuel Basket
  SAME AS FUEL BASKET 2
  IHSEL 15 17 18 19 20 21 22 23 24 25 26 27 28 29
  IFLINS 77 ! define the adjacent center insert heat sink
  IFLMCO 30 ! define the adjacent MCO wall heat sink
  END IHSEL for 3rd fuel basket
*
* 4th Fuel Basket
  SAME AS FUEL BASKET 2
  IHSEL 31 32 33 34 35 36 37 38 39 40 41 42 43 44
  IFLINS 79 ! define the adjacent center insert heat sink,
  IFLMCO 45 ! define the adjacent MCO wall heat sink
  IFLIAD 73 ! define the lid or floor heat sink to which the fuel
  ! radiate to
  FWEL0 0.9091 ! on the inner surface of the MCO wall
  FANEL0 0.01 ! wetted fraction of fuel surface
  FANELM 0.25 ! wetted fraction of MCO wall
  END IHSEL for 4th fuel basket
  END FUEL_BSKT
*
* SCRAP_BSKT 1 ! Total number of scrap baskets
*
* First scrap basket
  IHSSC 61 70 63 64 65 66 67 68 69 ! radial outward
*
  ISCONS 83 ! define the adjacent center insert heat sink,
  ! 0 for no insert, fin heat sink
  ISCYN 62 ! define the adjacent MCO wall heat sink
  ISCLD 71 ! define the adjacent MCO wall heat sink
  ISCLD 74 ! define the lid or floor heat sink to which the
  scrap ! radiate to
  * multiplier for effective conductivity in scrap basket in the order
  read in
  * (only conduction part)
  * FRSC 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
  * multiplier for effective conductivity in scrap basket in the order
  read in (radiation part)
  * (only radiation part)
  * FRSC 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
  * porosity of the scrap for each heat sink in the order read in

```

Date: 3/05/99

B - 34

```

FWEL0 0.0 ! on the inner surface of the MCO wall
FANEL 0.1 ! wetted fraction of fuel surface
FANELM 1.0 ! wetted fraction of MCO wall
HSELFL 1.16 ! mass of sludge particles (kg) in the fuel basket
! see comments on HSELFL above
*
* view factor matrix between the insert,
* outer surface of outer fuel elements,
* and the MCO wall. Therefore, the dimension of the square matrix is
* 1-number of fuel rods1. If there is no insert, number of fuel
  rods=1.
  FVIEW 0.000 0.926 0.074 0.000 0.000 0.000 0.000 0.000 0.000 0.000
  0.175 0.316 0.306 0.181 0.028 0.000 0.000 0.000 0.000 0.000
  0.014 0.306 0.306 0.306 0.028 0.014 0.000 0.000 0.000 0.000
  0.000 0.181 0.306 0.000 0.334 0.153 0.000 0.028 0.000 0.000
  0.000 0.014 0.153 0.167 0.153 0.153 0.153 0.167 0.028
  0.000 0.000 0.028 0.153 0.306 0.000 0.028 0.306 0.153
  0.000 0.000 0.014 0.153 0.306 0.000 0.306 0.153 0.348
  0.000 0.000 0.000 0.014 0.153 0.306 0.153 0.049 0.466
  0.000 0.000 0.000 0.000 0.035 0.115 0.220 0.590 0.040
  *
  * gap distance for micro-convection calculation
  XGAP 0.000 0.018 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
  0.018 0.000 0.021 0.021 0.073 0.000 0.000 0.000 0.000 0.000
  0.000 0.021 0.000 0.021 0.021 0.073 0.073 0.000 0.000 0.000
  0.000 0.021 0.021 0.000 0.000 0.021 0.021 0.000 0.021 0.083
  0.000 0.073 0.021 0.021 0.000 0.000 0.073 0.021 0.058
  0.000 0.000 0.073 0.000 0.021 0.000 0.073 0.021 0.026
  0.000 0.000 0.000 0.000 0.021 0.000 0.021 0.000 0.016
  0.000 0.000 0.000 0.073 0.021 0.021 0.021 0.000 0.016
  0.000 0.000 0.000 0.000 0.083 0.058 0.026 0.016 0.000
  *
  * axial conduction tracked in the fuel elements
  *
  * top to bottom axial partitions of the basket
  AXIAL 0.0521 0.0425 0.0648 0.0995 0.152 0.234 0.3551
  * multiplier to FMAXFL (fraction of geometric area exposed for
  * oxidation) for each axial basket. clad damage confined to the tip.
  * 1.0-0.0521=19.19 0.0 0.0 0.0 0.0 0.0
  * multiplier to FWEL0, FWEL10, and FWPM0 (initial amount of water per
  * geometric surface area of fuel, insert, and MCO wall) for each axial
  * basket. water on the tip of fuel. 1.0-0.0521=19.19
  * FWAX 19.19 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
  * multiplier to XFLOX0 (initial oxide/hydride thickness) for each axial
  * basket
  FUXAX 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
  * partition of HSELFL (mass of sludge particles) for each axial basket.
  FSLAX 0.0521 0.0425 0.0648 0.0995 0.152 0.234 0.3551
  END IHSEL for 1st fuel basket
*
* 2nd Fuel Basket
  *
  * SAME AS FUEL BASKET n* - duplicates the fuel basket data
  * SAME AS FUEL BASKET
  * any overriding parameters can be followed

```

FAI/98-40, Rev. 2

* multiplier for XDSCR(characteristic scrap size) for each axial basket
 FPDSC 1.0 1.0 1.0
 * multiplier for FXSC(multiplier for effective conductivity (conduction))
 in scrap) 0 1.0 1.0 1.0
 * multiplier for FRSC for effective conductivity (radiation)
 in scrap) 1.0 1.0 1.0 1.0
 END IHASC for 1st scrap basket
 END SCRAP_BSXT
 END MCO

Date: 3/05/99

B - 35

FAI/98-40, Rev. 2

FPOROS 0.40 0.40 0.40
 * character 0.685 0.685 0.685 0.685 0.685
 XDSCR 0.00635 0.00635 0.00635
 XSCGBK 0.0254 0.0254 0.0254 0.0254 0.0254
 XSCGBK 0.2842 1 radius of scrap basket (m)
 XSCBCK 0.676 1 height of scrap basket (m)
 * exposed surface area available for oxidation
 per unit volume of scrap (1/m) for each order read in.
 each scrap basket heat sink in the order read in.
 the values 125.63 125.63 125.63
 AVONSC 16.48 16.48 16.48 16.48 16.48
 XDHYSC 2.8-5 1 average diameter of hydride particle (m)
 FOXSC 10 0 1 multiplier for AVOXSC
 * Nominal hydride: 4% of exposed surface with multiplier of 300
 * NSCONOX*FSCHD = Fx * Fa * XDHYD / 6, where Fx is multiplier and Fa is area fraction
 = 0.04 + 300 + 2.E-5 / 6
 = 0.E-5
 * XSCOXO initial oxide thickness on the exposed surface (m)
 fraction of oxide which is hydride
 FSCHYD see fuel basket
 XSCOXO 4.OE-5 4.OE-5 4.OE-5 4.OE-5 4.OE-5
 4.OE-5 4.OE-5 4.OE-5
 FSCHYD 1.0 1.0 1.0 1.0 1.0
 1.0 1.0 1.0
 * 1.5 kg of water total for scrap basket; 1.5/0.1676 = 8.950 kg/m³
 MWVWSC 8.950 1 initial mass (kg) of water per unit bulk volume
 1/3 of scrap
 FNSCTO 0.0 1 on the outer surface of the insert
 FNSCHW 0.0 1 (per unit area, m²)
 1 on the inner surface of the MCO wall
 1 (per unit area, m²)
 FANSC 0.1 1 wetted fraction of surface area
 FANSCW 1.0 1 wetted fraction of MCO wall insert
 XSCINS 0.001 1 scrap actually located between
 XSCMCO 0.00635 1 mass of sludge particles (kg) in the scrap basket
 NSLSC 0.25 1 see comments on FVSL above
 * axial conduction tracked in the scrap basket, water on the bottom
 * 4 nodes, one 2- node at the bottom
 * top to bottom axial partition
 AXIAL 0.3083 0.3083 0.0751
 * multiplier for PFCOS (density of scrap) for each axial basket
 multipliers 1.0 1.0 1.0
 * multiplier for FOXSC(multiplier for oxidation area) for each axial basket
 FFOXSC 1.0 1.0 1.0
 * multiplier for MWVWSC(initial amount of water per unit volume) for each
 * axial basket. 1 kg on the bottom node, 0.167 kg on each of top three nodes.
 FVWSC 0.3605 0.3605 0.3605 8.877

B.5 Gas Property File

```

GAS NITROGEN      2.80130E+01    0.00000E+00
CVG 1.50000E+03    947.      7.42319E+02    -1.38235E-01    4.78640E-04    -2.57728E-07    4.14112E-11
BV 1.40000E+03    0.0001286    1.66786E-02    -5.33929E-01    -2.18321E+03    2.87500E+12    -1.65357E+14
PV 126.100E+00    3.3818E5    5.9826E1    -1.0976E3    -8.6689E0    4.6346E-2    1.0E0
HFG 300.      0.0E0    0.0E0    0.0E0    0.0E0    0.0E0    0.0E0
KG 0.026      0.0323    0.0383    0.044    0.0E0
MUG 1.5E3      5.3917E-5    7.632E-7    5.8823E-1    6.775E1    0.0E0
DFG 3.798      71.4      0.0E0
RL 300.      1.E-3      1.E-3      1.E0      1.E0      0.0E0      0.0E0
CVL 300.      1.E3      1.E3      0.0E0      0.0E0      0.0E0      0.0E0
*
GAS OXYGEN        3.20000E+01    0.00000E+00
CVG 1.50000E+03    881.      5.32655E+02    4.41600E-01    -1.54996E-04    4.29830E-09    4.29767E-12
BV 1.40000E+03    0.000871    1.21875E-03    -4.85625E-01    -2.65000E+03    5.12500E+12    -3.59375E+14
PV 154.580E+00    5.0416E6    5.2486E1    -1.2134E3    -6.7062E0    2.9764E-2    1.0E0
HFG 300.      0.0E0    0.0E0    0.0E0    0.0E0    0.0E0    0.0E0
KG 0.0263      0.0337    0.0410    0.0481    0.0E0
MUG 1.5E3      6.3987E-5    8.038E-7    6.0478E-1    7.03E1    0.0E0
DFG 3.467      106.7      0.0E0
RL 300.      1.E-3      1.E-3      1.E0      1.E0      0.0E0      0.0E0
CVL 300.      1.E3      1.E3      0.0E0      0.0E0      0.0E0      0.0E0
*
GAS STEAM         1.80000E+01    -2.41820E+08
CVG 1.57320E+03    2653.      1.33579E+03    -4.37917E-03    8.40632E-04    -4.06859E-07    6.03749E-11
BV 3.23000E+02    -0.04E0    2.29514E-3    -2.02444E+0    -8.77848E+5    -3.00507E+18    5.79857E+20
PV 647.290E+00    2.1977E7    7.25500E+01    -7.20670E+03    -7.13850E+00    4.04600E-06    2.0E0
HFG 300.E0      2.4376E6    3.18438E6    0.571707E0    -0.289795E0    -0.182469E0    0.295616E0
KG 0.0187      0.0271    0.0357    0.0471    0.0E0
MUG 370.E0      1.1946E-5    7.619E-8    9.2758E-1    2.116E2    -4.67E3
DFG 2.52E0      775.      1.0E0
RL 300.E0      1.E3      1.E3      1.E0      1.E0      0.0E0      0.0E0
CVL 300.E0      4200.E0      4200.E0      0.0E0      0.0E0      0.0E0      0.0E0
*
GAS HYDROGEN      2.00000E+00    0.00000E+00
CVG 4.00000E+02    14000.      1.05682E+04    -7.64315E-01    9.89067E-04    2.00916E-07    -5.85743E-11
BV 4.98000E+02    0.0E0      1.22500E-02    -1.42500E+00    -1.86500E+02    3.13500E+08    -3.77000E+09
PV 33.2500E+00    23.0300E+00    0.0E0    0.0E0    0.0E0    0.0E0    0.0E0
HFG 300.      0.0E0    0.0E0    0.0E0    0.0E0    0.0E0    0.0E0
KG 0.1869      0.2304    0.2304    0.2304    0.0E0
MUG 1.5E3      5.3917E-5    7.632E-7    5.8823E-1    6.775E1    0.0E0
DFG 3.798      71.4      0.0E0
RL 300.      1.E-3      1.E-3      1.E0      1.E0      0.0E0      0.0E0
CVL 300.      1.E3      1.E3      0.0E0      0.0E0      0.0E0      0.0E0
*
GAS HELIUM        4.00000E+00    0.00000E+00
CVG 4.00000E+02    3118.E0      3118.E0      0.0E0      0.0E0      0.0E0      0.0E0
BV 4.98000E+02    0.0E0      0.0E0      0.0E0      0.0E0      0.0E0      0.0E0
PV 33.2500E+00    23.0300E+00    0.0E0    0.0E0    0.0E0    0.0E0    0.0E0
HFG 300.      0.0E0    0.0E0    0.0E0    0.0E0    0.0E0    0.0E0
KG 0.1567      0.1906    0.2223    0.2524    0.0E0
MUG 1.5E3      5.3917E-5    7.632E-7    5.8823E-1    6.775E1    0.0E0
DFG 3.798      71.4      0.0E0
RL 300.      1.E-3      1.E-3      1.E0      1.E0      0.0E0      0.0E0
CVL 300.      1.E3      1.E3      0.0E0      0.0E0      0.0E0      0.0E0

```

**** USE FOR AS SERIES AEROSOL TESTS

```

* TCRT SET HIGH = 10***4
* VAPOR PRESSURE BY LN(10***5) = 11.5 = A + B/10***4
* LN(0.01) = -4.6 = A + B/100
* SO B = -16.1/.0099 = -1626, A=11.66
*
*
*

```

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GAS NA2O          62.0      0.00000E+00
CVG 300.      1000.E0      1000.E0      0.0E0      0.0E0      0.0E0      0.0E0
BV 300.      0.0E0      0.0E0      0.0E0      0.0E0      0.0E0      0.0E0
PV 1.E4      1.E5      11.66      -1626.E0      0.0E0      0.0E0      1.0E0
HFG 300.      0.0E0      0.0E0      0.0E0      0.0E0      0.0E0      0.0E0
RL 300.      2500.      2500.E0      0.0E0      0.0E0      0.0E0      0.0E0
CVL 300.      1.E3      1.E3      0.0E0      0.0E0      0.0E0      0.0E0
MUG 370.E0      1.1946E-5      7.619E-8      9.2758E-1      2.116E2      -4.67E3
DFG 2.52E0      775.      1.0E0

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**** CSOH USED FOR AEROSOL LEAKAGE VALIDATION
NOTE: KG IS OXYGEN VALUES

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GAS CSOH	149.91274	-2.59408E+08					
CVG 300.E0	276.5E0	2.12857E+02	3.33181E-01	-4.90431E-04	3.38981E-07	-8.44686E-11	
BV 300.	0.0	0.0	0.0	0.0	0.0	0.0	
PV 1.30619E+03	1.01325E6	4.18806E+01	-1.87360E+04	-3.83793E+00	3.16319E-04	-1.00000E+00	
HFG 298.E0	146.562E6	146.56E6	0.0	0.0	0.0	0.0	
RL 300.E0	1.E3	1.E3	1.E0	1.E0	0.E0	0.E0	
CVL 300.E0	4200.E0	4200.E0	0.E0	0.E0	0.E0	0.E0	
MUG 370.E0	1.1946E-5	7.619E-8	9.2758E-1	2.116E2	-4.67E3		
DFG 2.52E0	775.	1.0E0					
KG 0.0263	0.0337	0.0410	0.0481				

**** METHANOL USED FOR FOG VALIDATION

* NOTE MUG AND DFG VALUES ARE BOGUS, KG ARE HYDROGEN VALUES

GAS METHANOL	3.20420E+01	-2.00670E+08				
CVG 1.50000E+03	3280.	1.15417E+02	3.70061E+00	-1.54313E-03	2.61327E-07	-9.65537E-12
BV 2.56300E+02	-0.2867	-1.99738E-02	1.93496E+01	-3.34249E+06	2.40809E+19	-6.85787E+21
PV 512.58	8.0858E6	1.0993E2	-7.4713E3	-1.3988E1	1.5281E-2	1.0
HFG 175.59	1.289E6	1.239E6	-2.79E-1	5.08E-1	8.4E-2	0.E0
RL 300.	600.	600.E0	1.E0	1.E0	0.E0	0.E0
CVL 175.59	2214.	3.358E3	1.18782E1	3.0554E-2	0.E0	0.E0
MUG 370.E0	1.1946E-5	7.619E-8	9.2758E-1	2.116E2	-4.67E3	
DFG 2.52E0	775.	1.0E0				
KG 0.1869	0.2304	0.2304	0.2304			

**** CARBON DIO USED FOR FLOW & THERMODYNAMIC VALIDATION

* NOTE: KG IS OXYGEN VALUES

GAS CARBON DIO	4.40100E+01	-3.93520E+08				
CVG 1.50000E+03	1140.	2.84515E+02	1.55345E+00	-1.14113E-03	4.02762E-07	-5.30735E-11
BV 1.52100E+03	6.835E-4	1.23636E-03	-8.26136E-01	-3.44000E+04	1.95227E+15	-3.17500E+17
PV 204.E0	7.3617E6	8.55300E+01	-3.48130E+03	-1.13360E+01	2.15050E-02	1.0E0
HFG 300.	0.4E6	0.4E6	1.E0	0.E0	0.E0	0.E0
KG 0.0263	0.0337	0.0410	0.0481			
MUG 1500.	5.2032E-5	2.148E-6	4.6E-1	2.9E2	0.E0	
DFG 3.941	195.2	0.E0				
RL 300.	0.4E6	0.77E3	1.E0	1.E0	0.E0	0.E0
CVL 300.	0.4E6	800.E0	0.E0	0.E0	0.E0	0.E0

*GAS PUO2OH2	308.	-1.0E8				
*CVG 300.E0	1000.0	1000.0	0.0	0.0	0.0	0.0
*BV 300.	0.0	0.0	0.0	0.0	0.0	0.0
*PV 1.0E5	1.01325E6	-46.0	0.0	0.0	0.0	0.0
*HFG 298.E0	1.0E6	1.0E6	0.0	0.0	0.0	0.E0
*RL 300.E0	1.E3	1.E3	1.E0	1.E0	0.E0	0.E0
*CVL 300.E0	4200.E0	4200.E0	0.E0	0.E0	0.E0	0.E0
*MUG 370.E0	1.1946E-5	7.619E-8	9.2758E-1	2.116E2	-4.67E3	
*DFG 2.52E0	775.	1.0E0				

* 'GAS' WATER IS DEFINED TO MIMIC THE THERMAL PROPERTIES (HEAT TRANSFER AND

* THERMAL CAPACITY) OF THE WATER IN THE GAP BETWEEN MCO AND CASK

GAS WATER	31000.	-3.93520E+08				
CVG 323.15	4180.	4180.	0.	0.	0.	0.
BV 323.15	0.000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
PV 204.E0	7.3617E6	8.55300E+01	-3.48130E+03	-1.13360E+01	2.15050E-02	1.0E0
HFG 300.	2.4E6	2.4E6	0.E0	0.E0	0.E0	0.E0
KG 0.64	0.68	0.68	0.60			
MUG 323.15	54.71E-5	54.71E-5	0.	0.	0.	
DFG 3.941	195.2	0.E0				
RL 300.	1000.	1000.	0.E0	1.E0	0.E0	0.E0
CVL 300.	4180.	4180.	0.E0	0.E0	0.E0	0.E0

APPENDIX C
SAMPLE PROBLEM OUTPUT

C.1	Cold Vacuum Drying	C-2
C.2	MCO Shipping	C-5
C.3	MCO Staging	C-8
C.4	Cold Vacuum Drying With Axial Variation in Fuel Damage	C-11

APPENDIX C
SAMPLE PROBLEM OUTPUT

C.1 Cold Vacuum Drying

CVD2VNH: Vacuum Cycle, Bounding Area, Nominal Hydride

CVD2VNH: Vacuum Cycle, Bounding Area

Nominal Hydride

APPENDIX C
SAMPLE PROBLEM OUTPUT

C.2 MCO Shipping

Shipping, 770 W MCO, Hanford Hottest Day

Shipping, 770 W MCO, Hanford Hottest Day

APPENDIX C
SAMPLE PROBLEM OUTPUT

C.3 MCO Staging

STAGING, 770 W MCO, 108 C MCO Wall Temp.

STAGING, 770 W MCO, 108 C MCO Wall Temp.

APPENDIX C
SAMPLE PROBLEM OUTPUT

C.4 Cold Vacuum Drying With Axial Variation in Fuel Damage

VCIAXF: CVD Vac+He FFFFS U=10 UH3=12 H2O=20.6

VC1AXF: CVD Vac+He FFFFS U=10 UH3=12 H2O=20.6

VC1AXF: CVD Voc+He FFFFS U=10 UH3=12 H2O=20.6

APPENDIX D
QUALITY ASSURANCE DOCUMENTS

Included here are:

1. Calculation Note Cover Sheet.
2. Authorship and Reviewer Table.
3. Calculation Note Methodology Checklist.

CALCULATION NOTE COVER SHEET

SECTION TO BE COMPLETED BY AUTHOR(S):

Calc Note Number <u>FAI/98-40</u>		Revision Number <u>2</u>	Page <u>1</u> to <u>D-4</u>
Title <u>Hanford Spent Nuclear Fuel Safety Analysis Model HANSE 1.3: User's Manual</u>			
Project <u>Hanford Spent Nuclear Fuel</u>	Project Number or Shop Order <u>EDN001-14</u>		
Purpose: Describe phenomena, models, utilization, validation, and results of HANSE 1.3; revise test case for minor revision 1.3.1.			
Results Summary: Purpose is achieved.			
References of Resulting Reports, Letters, or Memoranda (Optional)			
<hr/>			
Author(s): (See Page D-3)			Completion
Name (Print or Type)	Signature	Date	
<u>Sung Jin Lee</u>	<u>Sung Jin Lee</u>	<u>3/05/99</u>	
<u>Martin G. Plys</u>	<u>(Rev. 0 Author) N/A on this Rev.</u>	<u>N/A</u>	
<u>Boro Malinovic</u>	<u>(Revs. 0 & 1 Author) N/A on this Rev.</u>	<u>N/A</u>	
<u>Michael Epstein</u>	<u>(Rev. 0 Author) N/A on this Rev.</u>	<u>N/A</u>	

SECTION TO BE COMPLETED BY VERIFIER(S):

Verifier(s): (See Page D-3)			Completion
Name (Print or Type)	Signature	Date	
<u>Martin G. Plys</u>	<u>M. Plys</u>	<u>3/05/99</u>	
<u>Boro Malinovic</u>	<u>(Rev. 0 Verifier) N/A on this Rev.</u>	<u>N/A</u>	
<u>Sung Jin Lee</u>	<u>(Rev. 0 Verifier) N/A on this Rev.</u>	<u>N/A</u>	
Independent Review or			
Method of Verification: Design Review <u> </u> , Alternate Calculations <u>X</u> , Testing <u> </u>			
Other (specify) <u> </u>			

SECTION TO BE COMPLETED BY MANAGER:

Responsible Manager:		Approval Date
Name (Print or Type)	Signature	
<u>Martin G. Plys</u>	<u>M. Plys</u>	<u>03/05/99</u>

Rev. 2 changes were authored by Sung Jin Lee and reviewed by M.G Plys.

Rev. 1 changes were authored by B. Malinovic and reviewed by M.G Plys. Authorship and review of Rev. 0 is as follows:

Section	Author	Reviewer
1	M.G. Plys	B. Malinovic & S.J. Lee
2	M.G. Plys	B. Malinovic & S.J. Lee
3.1 - 3.2	M.G. Plys	B. Malinovic & S.J. Lee
3.3 - 3.10	S.J. Lee	B. Malinovic & M.G. Plys
3.7.2	M. Epstein	M.G. Plys
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5	B. Malinovic	S.J. Lee & M.G. Plys
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7	B. Malinovic	S.J. Lee & M.G. Plys
8	B. Malinovic	S.J. Lee & M.G. Plys
9	B. Malinovic	S.J. Lee & M.G. Plys
App. A	B. Malinovic	S.J. Lee & M.G. Plys
App. B	B. Malinovic	S.J. Lee & M.G. Plys
App. C	B. Malinovic	S.J. Lee & M.G. Plys
App. D	N/A	N/A

CALC NOTE NUMBER FAI/98-40 REV. 2 PAGE i to D-4

CALCULATION NOTE METHODOLOGY CHECKLIST

CHECKLIST TO BE COMPLETED BY AUTHOR(S) (CIRCLE APPROPRIATE RESPONSE)

1. Is the subject and/or the purpose of the design analysis clearly stated? YES . NO
2. Are the required inputs and their sources provided? YES . NO . N/A
3. Are the assumptions clearly identified and justified? YES . NO . N/A
4. Are the methods and units clearly identified? YES . NO . N/A
5. Have the limits of applicability been identified? YES . NO . N/A
(i.e., Is the analysis for a 3 or 4 loop plant or for a single application.)
6. Are the results of literature searches, if conducted, or other background data provided? YES . NO . N/A
7. Are all the pages sequentially numbered and identified by the calculation note number? YES . NO
8. Is the project or shop order clearly identified? YES . NO
9. Has the required computer calculation information been provided? YES . NO . N/A
10. Were the computer codes used under configuration control? YES . NO . N/A
11. Was the computer code(s) used applicable for modeling the physical and/or computational problems identified? YES . NO . N/A
(i.e., Is the correct computer code being used for the intended purpose.)
12. Are the results and conclusions clearly stated? YES . NO
13. Are Open Items properly identified? YES . NO . N/A
14. Were approved Design Control practices followed without exception? YES . NO . N/A
(Approved Design Control practices refers to guidance documents within NSD that state how the work is to be performed, such as how to perform a LOCA analysis.)
15. Have all related contract requirements been met? YES . NO . N/A

NOTE: If NO to any of the above, Page Number containing justification _____