OCT 10 1996

ENGINEERING DATA TRANSMITTAL

Page 1 of 1

1. EDT

No 614692

2. To: (Receiving Organization) Distribution		3. From: (Originating Organization) Process Engineering Analysis		4. Related EDT No.: N/A	
5. Proj./Prog./Dept./Div.: 74A50		6. Cog. Engr.: F. J. Heard		7. Purchase Order No.: N/A	
8. Originator Remarks: Approval/Release				9. Equip./Component No.: N/A	
				10. System/Bldg./Facility: N/A	
11. Receiver Remarks:				12. Major Assm. Dwg. No.: N/A	
				13. Permit/Permit Application No.: N/A	
				14. Required Response Date:	

15. DATA TRANSMITTED					(F)	(G)	(H)	(I)
(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	Approval Desig- nator	Reason for Trans- mittal	Orig- inator Dispo- sition	Receiv- er Dispo- sition
1	WHC-SD-SNF-ER-012		0	Thermal Hydraulic Feasibility Assessment of the Hot Conditioning System and Process	N/A	1	1	

16. KEY							
Approval Designator (F)		Reason for Transmittal (G)			Disposition (H) & (I)		
E, S, Q, D or N/A (see WHC-CM-3-5, Sec.12.7)		1. Approval	4. Review		1. Approved	4. Reviewed no/comment	
		2. Release	5. Post-Review		2. Approved w/comment	5. Reviewed w/comment	
		3. Information	6. Dist. (Receipt Acknow. Required)		3. Disapproved w/comment	6. Receipt acknowledged	

17. SIGNATURE/DISTRIBUTION (See Approval Designator for required signatures)									
(G)	(H)	(J) Name	(K) Signature	(L) Date	(M) MSIN	(J) Name	(K) Signature	(L) Date	(M) MSIN
Reason	Disp.								
1	1	Cog.Eng. F. J. Heard	<i>F. J. Heard</i>	10/2/96	H0-34				
1	1	Cog. Mgr. D. M. Ogden	<i>D. M. Ogden</i>	10/2/96	H0-34				
		QA							
		Safety							
		Env.							
1	1	J. R. Frederickson	<i>J. R. Frederickson</i>	10/4/96	R3-86				

18. Signature of EDT Originator <i>F. J. Heard</i> Date <i>10/2/96</i>		19. Authorized Representative Date for Receiving Organization C. R. Miska <i>C. R. Miska</i> Date <i>10-8-96</i>		20. Cognizant Manager Date <i>D. M. Ogden</i> Date		21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments	
---	--	--	--	--	--	---	--

Thermal Hydraulic Feasibility Assessment of the Hot Conditioning System and Process

F. J. Heard

LMHC Westinghouse Hanford Company, Richland, WA 99352

U.S. Department of Energy Contract ~~DE-AC06-87RL10930~~ 80232764-9-K001

EDT/ECN: 614692

UC: 2020

Org Code: 74A50

Charge Code: LB040

B&R Code: EW3135040

Total Pages: 234

Key Words: Spent Nuclear Fuel, K Basins, Thermal Hydraulic, Chemical Reactions, Corrosion, Finite Element Methods, Models, Temperature Control, Multi-Canister Overpak, Technical Acquisition Program, Scoping Analyses, Path Forward, Integrated Process Strategy, Hydride Decomposition, Passivation, Hot Conditioning

Abstract: A series of analyses have been completed investigating the thermal hydraulic performance and feasibility of the Hot Conditioning Process (HCS) for the Spent Nuclear Fuel Project (SNFP). The SNFP was established to develop engineered solutions for the expedited removal, stabilization, and storage of spent nuclear fuel from the K Basins at the U.S. Department of Energy's Hanford Site in Richland, Washington. The subject efforts focus on independently investigating, quantifying, and establishing the governing heat production and removal mechanisms for each of the HCS operations and configurations, obtaining preliminary results for comparison with and verification of other analyses, and providing technology-based recommendations for consideration and incorporation into the HCS design bases. The goal is to develop a series of thermal-hydraulic models that could respond to all process and safety-related issues that may arise pertaining to the HCS. A series of sensitivity analyses were also performed to help identify those parameters that have the greatest impact on energy transfer and, hence, temperature control. It is anticipated that the subject thermal-hydraulic models will form the basis for a series of advanced and more detailed models that will more accurately reflect the thermal performance of the HCS and alleviate the necessity for some of the more conservative assumptions and oversimplifications, as well as form the basis for the final process and safety analyses.

TRADEMARK DISCLAIMER. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors.

Printed in the United States of America. To obtain copies of this document, contact: WHC/BCS Document Control Services, P.O. Box 1970, Mailstop H6-08, Richland WA 99352, Phone (509) 372-2420; Fax (509) 376-4989.

James Bishop 10-10-96
Release Approval

Date

Release Stamp

Approved for Public Release

Thermal Hydraulic Feasibility Assessment of the
Hot Conditioning System and Process

T. R. Beaver
F. J. Heard
Westinghouse Hanford Company

M. J. Thurgood
John Marvin, Inc.
Prepared for Westinghouse Hanford Company

September 1996

Issued by
WESTINGHOUSE HANFORD COMPANY
for the

U.S. DEPARTMENT OF ENERGY
RICHLAND OPERATIONS OFFICE
RICHLAND, WASHINGTON

**THERMAL HYDRAULIC FEASIBILITY ASSESSMENT OF THE
HOT CONDITIONING SYSTEM PROCESS**

**T. R. Beaver
F. J. Heard
Westinghouse Hanford Company**

**M. J. Thurgood
John Marvin, Inc.**

ABSTRACT

The Spent Nuclear Fuel Project was established to develop engineered solutions for the expedited removal, stabilization, and storage of spent nuclear fuel from the K Basins at the U.S. Department of Energy's Hanford Site in Richland, Washington. A series of analyses have been completed investigating the thermal-hydraulic performance and feasibility of the proposed Hot Conditioning System and process for the Spent Nuclear Fuel Project. The analyses were performed using a series of thermal-hydraulic models that could respond to all process and safety-related issues that may arise pertaining to the Hot Conditioning System. The subject efforts focus on independently investigating, quantifying, and establishing the governing heat production and removal mechanisms, flow distributions within the multi-canister overpack, and performing process simulations for various purge gases under consideration for the Hot Conditioning System, as well as obtaining preliminary results for comparison with and verification of other analyses, and providing technology-based recommendations for consideration and incorporation into the Hot Conditioning System design bases.

EXECUTIVE SUMMARY

A series of analyses have been completed investigating the thermal-hydraulic performance and feasibility of the hot conditioning system (HCS) and process.

The subject analyses focus on quantifying the internal flow distributions within the multi-canister overpack (MCO), establishing the governing energy production and removal capabilities during the Hot Conditioning System (HCS) process steps, and performing process simulations for the various purge gases under consideration. The goal is to develop a series of thermal-hydraulic models that could respond to all process and safety related issues that may arise pertaining to the HCS, as well as obtain preliminary results for comparison with and verification of other analyses and provide technology-based recommendations for consideration by the HCS design authorities.

The results of the flow analyses are as follows:

1. The socketed base plate design does much better at distributing an even flow to the fuel assemblies, but still has approximately 14 to 21% bypass flow depending on the fuel type. The socketed base plate design is recommended for the Mark Ia and Marl IV fuel baskets.
2. The scrap basket, because of the high flow resistance associated with a porous media, was initially estimated to have 46% bypass

flow. Flow restrictors, within the annulus between the scrap basket skirt and the MCO inner diameter, decrease the bypass flow to 13-20% of the total MCO gas flow. Annular flow restrictors are recommended for both the scrap and fuel baskets to maximize the amount of flow passing through the various baskets, during the passivation phase, to prevent the higher oxygen concentration within the bypass flow from obscuring the true oxygen concentration as measured by the process instrumentation.

3. Additional design work may be required to limit flow channeling through partially or unevenly filled fuel or scrap baskets. One possible design modification for consideration involves reducing the number and spacing of the flow holes through the scrap basket baseplate. This would result in the baseplate becoming the controlling resistance rather than the porous media and would minimize flow redistribution or flow channeling within a partially or unevenly filled scrap basket. The use of dummy fuel elements to completely load out a fuel basket may be a simple solution to effectively reduce flow channeling within a partially filled fuel basket.

The following thermal results, conclusions, and recommendations are based on nominal chemical reaction rate relationships associated with unirradiated and uncorroded uranium metal with oxygen, a conservative estimate of the total reactive surface area of 800000 cm² for each scrap basket, and the conservative assumption that the upper six inches of each fuel assembly is completely declad. (NOTE: The above reactive surface areas are associated

with the safety bases for the spent nuclear fuel project (SNFP)). The results of the thermal analyses indicate that careful consideration will need to be given to the location and variation of fuel temperatures within the MCO during the HCS passivation process to insure that:

1. Sufficient and a uniform distribution of oxygen reaches all exposed fuel surfaces such that highly reactive uranium metal is not left unpassivated in the MCO. This could occur if highly damaged fuel in the lower elevations of the MCO consume all the oxygen before it reaches the upper elevations of the MCO preventing fuel in the upper baskets from being passivated. This process may not be controllable for highly damaged fuel or scrap, since any reaction that starts will continue as oxygen continues to be added to the system or until all of the oxygen is consumed.

2. The chemical heat of reaction will be the dominate heat source at higher fuel temperatures and/or increased oxygen concentrations. This may lead to the fuel temperatures that could potentially exceed the alpha-beta phase change temperature leading to cladding failure and the extrusion of fuel into the flow channels, thereby increasing the reactive surface area many times and increasing the local reaction rate. Such a scenario may cause the fuel to melt during the passivation process step. An atmospheric ingress accident with 21% oxygen by volume will lead to a large energy spike and potentially excessive temperatures. A safety significant confinement system, a safety class confinement system, or an emergency inert gas blanketing system for the MCO, dewar

flow annulus, and the HCS vacuum chamber, depending on the results of a probabilistic safety analysis (PRA), may be required to mitigate the consequences of an oxygen ingress accident and allow the chemical energy to slowly dissipate.

3. The high reaction heat, coupled with low heat removal capability, may also make the process hard to control. Hot spots within the MCO will be difficult to detect by the process instrumentation given the thermal time constant of the fuel, heat transfer to adjacent fuel assemblies or MCO structures, and the potential for significant oxygen bypass.
4. The presence of radial and axial temperature profiles in the fuel during passivation are likely to result in non-uniform oxygen consumption which will result in local hot spots.

Other findings are summarized as follows;

1. The use of helium, rather than argon, as the HCS process purge gas can significantly reduce the heatup and cooldown times and is recommended as the purge gas of choice for the HCS process. The proposed 12 hour HCS cooldown is not adequate for either argon or helium. Significant temperature gradients exist within the MCO, especially during the 12 hour HCS cooldown period prior to commencing the passivation phase, that could result in local temperatures sufficiently high enough to produce a chemically reactive hot spot given the oxygen feed during the passivation

phase. A minimum of a 12 hour extension beyond the 12 hour HCS cooldown period, while holding at an inlet temperature of 423.16 ° F (302 °F), appears to provide adequate time given helium as the purge gas to minimize the temperature gradients within the scrap basket prior to commencing the passivation phase. A hold time longer than 12 hours will be required for fuel baskets, given that the effective thermal resistance of the scrap basket is less than the fuel baskets, but has not yet been investigated. (Much longer hold times will be required for argon under any condition.) Any modification to the proposed HCS process times must be adequately investigated for thermal impacts on both the scrap and fuel baskets.

2. The presence of two scrap baskets (top and bottom) within an MCO leads to a set of unique thermal concerns. These are:
 - a. At the proposed inlet temperature of 150 °C (302 °F) the lower scrap basket will consume all the oxygen within the first few inches resulting in excessive temperatures (> 1000 °F). Reducing the inlet temperature by 50 °C allows oxygen to pass through the lower scrap basket to higher levels, but the increase in purge gas temperature as it reaches the upper scrap basket, produces the same temperature excursion in the upper basket as occurred in the lower basket.
 - b. A single chemically active "hot spot" within the scrap or fuel baskets will eventually lead to excessive temperatures. A "hot and cold spot" analysis given

statistical variations in the decay heat, reactive surface area multiplier, the geometrical area-to-volume ratio, and scrap basket local porosity has not yet been initiated.

- c. Currently planned process instrumentation may not be able to determine if the oxygen is being consumed on an distributed or localized "hot spot" basis. The purge gas flow from the MCO, as measured by the process instrumentation, could have a significant oxygen concentration due to sufficient bypass flow around the scrap and socketed fuel basket designs, while the remainder of the oxygen has been consumed in a very local area producing excessive fuel temperatures. It will be difficult to detect such local hot spots. As previously recommended, bypass flow should be minimized by using flow restrictors on both the scrap and fuel baskets. Other possible designs to minimize bypass flow include full length skirts that will intersect with each tier and a seal ring around the upper perimeter of the lower spider assembly.
- d. The process instrumentation may not be adequate to detect the increase in purge gas temperature associated with a "hot spot", due to the long thermal time constant of the fuel or heat transfer to adjacent fuel and/or MCO internals.

3. A single upper scrap basket is recommended.
4. Given the potential variability in MCO contents, the HCS process operational strategies should be designed to allow for variable (0 - 5%) rather than a constant oxygen concentration and a variable helium purge gas flow rate (to be determined) that would help to minimize the radial and axial temperature gradients.
5. The above conclusions and recommendations assume conservative surface areas and published reaction rate relationships based on unirradiated and uncorroded uranium metal. Characterization data based on actual K Basin fuel is needed in these areas.

In summary, a uniform distribution of oxygen will be hard to achieve. Chemically active "hot spots" leading to excessive temperatures can occur via local variations in reactive surface area, temperature gradients, and oxygen concentrations. Additional model development and analyses are recommended to investigate combinations of scrap and fuel baskets within a MCO; such as, a less than the full complement of baskets, or a single upper or lower scrap and four fuel baskets, or five fuel and no scrap baskets. The following analyses are strongly recommended: (1) investigate the effects of decreased reactive surface areas, reaction rate relationships based on actual characterization data, variable process flow rates, a variable oxygen concentration feed during the passivation phase, and vacuum conditions, (2) investigate the effects of "statistical" based non-uniform distributions for decay heat, reactive surface areas, and scrap basket porosity, and (3) determine a modified HCS process heatup and/or cooldown rate, that could, respectively, in the minimum amount

of time, obtain the minimum temperature necessary for complete dehydriding and reduce the temperature gradients within the MCO prior to commencing the passivation phase. Items #1 and #2 must be performed to support the safety analysis report (SAR) and the final HCS design. (Item #2 is especially important when investigating the effects of chemically active "hot and cold spots" given a more realistic treatment of the variations expected with actual MCO loadings.) Item #3 must be performed to support HCS process operations given a final design or the assumed "statistical" variations in MCO loadings.

CONTENTS

1.0	INTRODUCTION	1-1
1.1	PURPOSE AND SCOPE	1-1
1.2	BACKGROUND AND OBJECTIVES	1-2
1.3	HOT CONDITIONING SYSTEM AND PROCESS DESCRIPTION	1-2
2.0	SUMMARY	2-1
3.0	MODEL DEVELOPMENT, METHODOLOGY, AND ASSUMPTIONS	3-1
3.1	STATUS OF THERMAL MODELING	3-1
3.2	TECHNICAL ISSUES	3-2
3.2.1	Reaction Rates	3-3
3.2.2	Thermo-physical Properties, Effective Thermal Conductivity and Convective Heat Transfer Coefficients	3-5
3.2.3	Mass Transport	3-7
3.3	FLOW DISTRIBUTION AND BASKET DESIGN	3-7
3.3.1	Network Flow Distribution Models	3-8
3.3.2	Three-Dimensional MCO Flow Model	3-11
3.4	MCO PASSIVATION MODELS	3-13
3.4.1	One-Dimensional Scoping Models	3-13
3.4.2	Three-Dimensional Integrated MCO Model	3-21
3.5	MCO HOT CONDITIONING MODEL	3-22
3.5.1	Three-Dimensional Detailed Single Tier Models	3-22
3.5.2	Three-Dimensional MCO Simple Ring Model	3-26
4.0	RESULTS	4-1
4.1	FLOW DISTRIBUTION VERSUS BASKET DESIGN	4-1
4.1.1	Mark IA Baskets	4-1
4.1.2	Mark IV Baskets	4-2
4.1.3	Scrap Basket	4-4
4.2	MCO SUB-CHANNEL FLOW DISTRIBUTION	4-6
4.3	PASSIVATION REACTION LENGTH	4-8
4.3.1	Reaction Length for Complete Consumption of Oxygen	4-8
4.3.2	Heat Release Due to Oxidation Reaction	4-9
4.3.3	Time to Achieve Reaction Depth	4-9
4.4	HCS THERMAL-HYDRAULIC PERFORMANCE	4-11
4.4.1	Process Simulation With Integrated COBRA-TF Model	4-11
4.4.2	Process Simulation With Simplified COBRA-TF Model	4-14
4.4.3	Scrap Basket Thermal Performance and Process Simulation With Detailed Tier Model	4-15
5.0	CONCLUSIONS AND RECOMMENDATIONS	5-1

LIST OF FIGURES

1-1.	Process Flow for the Spent Nuclear Fuel Project	1-5
1-2.	Process Times for the Hot Conditioning System	1-6
3-1.	Perforated Plate Basket Design for Mark Ia Fuel	3-29
3-2.	Socket Basket Design for Mark Ia Fuel	3-30
3-3.	Hydraulic Network for Perforated Plate Type Fuel Baskets	3-31
3-4.	Hydraulic Network for Socket Type Fuel Baskets	3-32
3-5.	Wire Mesh Basket Design for Mark IV Fuel	3-33
3-6.	Hydraulic Network for Wire Mesh Type Fuel Baskets	3-34
3-7.	Cross Section View of Scrap and Mark IV Fuel Assembly Baskets	3-35
3-8.	MCO Configuration for Integrated Model.	3-36
3-9.	COBRA-TF Model of MCO.	3-37
3-10.	Vertical Flow Channels for Fuel Assembly Storage Basket.	3-38
3-11.	Lateral Channels for Fuel Assembly Storage Basket.	3-39
3-12.	Comparison of the Ritchie and Pearce Reaction Rate Relationships in Dry Air versus Temperature	3-40
3-13a.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 21% Oxygen by Volume in Dry Air	3-41
3-13b.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 10% Oxygen by Volume in Dry Air	3-41
3-13c.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 5% Oxygen by Volume in Dry Air	3-42
3-13d.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 4% Oxygen by Volume in Dry Air	3-42
3-13e.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 3% Oxygen by Volume in Dry Air	3-43
3-13f.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 2% Oxygen by Volume in Dry Air	3-43
3-13g.	Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 1% Oxygen by Volume in Dry Air	3-44
3-14.	Reaction Rate in Dry Air versus Temperature for Different O ₂ Volume Fractions	3-45
3-15.	Conceptual Design of Hot Conditioning System Containing a MCO Shown Without Shield Plug and HCS Upper Components	3-46
3-16.	Representative Flow Patterns for Lower Scrap Basket Within MCO at the HCS Station	3-47
3-17.	Planar View of the 30° Sector Model of a MCO Tier Containing Mark IV Fuel Assemblies Within the HCS	3-48
3-18.	Planar View of the 30° Sector Model of a MCO Tier Containing Scrap Fuel Within the HCS	3-49
3-19.	Three-Dimensional Isometric View of a 30° Sector Model of a MCO Tier Containing Mark IV Fuel Assemblies Within the HCS	3-50
3-20.	Three-Dimensional Isometric View of a 30° Sector Model of a MCO Tier Containing Scrap Fuel Within the HCS	3-51
3-21.	Nodalization Pattern for Three-Dimensional Fuel Basket Tier Model	3-52
3-22.	Nodalization Pattern for Three-Dimensional Scrap Basket Tier Model	3-53
3-23.	Effective Thermal Conductivity Based on Hadley's Correlation for Uranium Metal and Various Carrier Gases for Porosities of 0.259 and 0.476	3-54
3-24.	Ring Model for Simplified Three-Dimensional MCO COBRA-TF Model	3-55

3-25.	Blow Up of Ring Model for Simplified Three-Dimensional MCO COBRA-TF Model	3-56
3-26.	Comparison of Radial Temperature Gradient From Simplified COBRA-TF Model versus Analytical Solution	3-57
4-1.	Scrap Basket Bypass Flow for Intact Fuel Elements	4-21
4-2.	Scrap Basket Bypass Flow for Fuel Assembly Outer Elements	4-22
4-3.	Vertical Velocity in Rubble and Fuel Central Channels	4-23
4-4.	Vertical Velocity in Rubble and Fuel Annular Channels	4-24
4-5.	Vertical Velocity in Rubble and Fuel Exterior Central Channels	4-25
4-6.	Vertical Velocity in Rubble and Fuel Exterior Edge Channels	4-26
4-7.	Length for Complete Reaction Versus Temperature for an Argon Gas Flow of 10 CFM and Reaction Area Equal to That of Declad Fuel Using Modified Ritchie for Oxygen Concentrations from 0.1% to 2.5% by Volume	4-27
4-8.	Length for Complete Reaction Versus Temperature for an Argon Gas Flow of 10 CFM and Reaction Area Equal to 800,000 cm ² Using Modified Ritchie for Oxygen Concentrations from 0.1% to 2.5% by Volume	4-28
4-9.	Length for Complete Reaction Versus Temperature for a Nitrogen Gas Flow of 10 CFM and Reaction Area Equal to 10X That of Declad Fuel Using Modified Ritchie for Oxygen Concentrations from 0.1% to 2.5% by Volume	4-29
4-10.	Length for Complete Reaction Versus Reaction Surface Area for a Gas Flow of 10 CFM and Fuel Temperature of 473 °K (200 °C) Based on Modified Ritchie	4-30
4-11.	Lineal Heat Generation Rate Due to Oxygen Oxidation Reaction Versus Fuel Temperature Based on Ritchie	4-31
4-12.	Total Heat Generation Rate for Complete Reaction of Available Oxygen Versus Pump Volumetric Flow Given an Exit Fuel Temperature of 473 °K (200 °C)	4-32
4-13a.	Heating Rate Assuming All Reaction Energy is Deposited in the Fuel for a Constant 2% Oxygen Concentration.	4-33
4-13b.	Heat Rate Assuming All Reaction Energy is Deposited in the Fuel for the Complete Consumption of Various Oxygen Concentrations	4-33
4-14.	Time to React Fuel to a Specified Depth as a Function of Temperature for a Reaction Area Equal to that of Declad Fuel Using Modified Ritchie Assuming a Constant 2% Oxygen Concentration	4-34
4-15.	Time to React Fuel to a Specified Depth as a Function of Temperature for a Reaction Area Equal to 10X that of Declad Fuel Using Modified Ritchie Assuming a Constant 2% Oxygen Concentration	4-35
4-16.	Gas Temperature in Rubble and Fuel Central Channels (Time = 30 Hours)	4-36
4-17.	Gas Temperature in Rubble and Fuel Exterior Channels (Time = 30 Hours)	4-37
4-18.	Gas Temperature in Rubble and Fuel Exterior Edge Channels (Time = 30 Hours)	4-38
4-19.	Temperature of Rubble Basket (Time = 30 Hours)	4-39
4-20.	Temperature of Central Elements (Time = 30 Hours)	4-40
4-21.	MCO Structure Temperatures (Time = 30 Hours)	4-41

4-22.	Oxygen Volume Fraction in Rubble and Fuel Exterior Central Channels (Time = 30 Hours)	4-42
4-23.	Oxygen Volume Fraction in Rubble and Fuel Exterior Edge Channels	4-43
4-24.	Gas Temperature in Rubble and Central Channels (Time = 34 Hours)	4-44
4-25.	Oxygen Volume Fraction in Rubble and Fuel Exterior Channels (Time = 34 Hours)	4-45
4-26.	Gas Temperature in Rubble and Fuel Central Channels (Time = 40 Hours)	4-46
4-27.	Gas Temperature in Rubble and Fuel Exterior Central Channels (Time = 40 Hours)	4-47
4-28.	Gas Temperature in Rubble and Fuel Exterior Edge Channels (Time = 40 Hours)	4-48
4-29.	Temperature of Rubble Basket (Time = 40 Hours)	4-49
4-30.	Temperature of Central Fuel Elements (Time = 40 Hours)	4-50
4-31.	MCO Structure Temperatures (Time = 40 Hours)	4-51
4-32.	Oxygen Volume Fraction in Rubble and Fuel Central Channels (Time = 40 Hours)	4-52
4-33.	Oxygen Volume Fraction in Rubble and Fuel Exterior Edge Channels (Time = 40 Hours)	4-53
4-34.	Gas Temperature in Rubble and Fuel Central Channels (Time = 40 Hours)	4-54
4-35.	MCO Rod and Structure Temperature for the Second Basket from the Bottom During Heat Up Using Helium for an Average Powered MCO	4-55
4-36.	MCO Rod and Structure Temperature for the Second Basket from the Bottom During Heat Up Using Argon for an Average Powered MCO	4-56
4-37.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 0.5% by Volume	4-57
4-38.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 1.0% by Volume	4-58
4-39.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 1.5% by Volume	4-59
4-40.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 2.0% by Volume	4-60
4-41.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 3.0% by Volume	4-61
4-42.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 4.0% by Volume	4-62
4-43.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 5.0% by Volume	4-63
4-44.	Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 10.0% by Volume	4-64
4-45.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 0.5% by Volume	4-65

4-46.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 1.0% by Volume	4-66
4-47.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 1.5% by Volume	4-67
4-48.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 2.0% by Volume	4-68
4-49.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 3.0% by Volume	4-69
4-50.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 4.0% by Volume	4-70
4-51.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 5.0% by Volume	4-71
4-52.	Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 10.0% by Volume	4-72
4-53.	Temperature Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 0.5% by Volume	4-73
4-54.	Temperature Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 1.0% by Volume	4-74
4-55.	Oxygen Mass Fraction Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 0.5% by Volume	4-75
4-57.	Temperatures Versus Time During 72 Hour HCS Simulation for Various Nodes Within a Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-77
4-58.	Temperatures Versus Time During Heatup Phase of HCS Simulation for Various Nodes Within a Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-78
4-59.	Temperatures Versus Time During Cooldown Phase of HCS Simulation for Various Nodes Within a Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-79
4-60.	Temperatures Contour Plot at 3 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-80
4-61.	Temperatures Contour Plot at 6 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-81
4-62.	Temperatures Contour Plot at 9 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-82
4-63.	Temperatures Contour Plot at 12 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-83
4-64.	Temperatures Contour Plot at 36 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-84

4-65.	Temperatures Contour Plot at 60 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-85
4-66.	Temperatures Contour Plot at 63 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-86
4-67.	Temperatures Contour Plot at 66 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-87
4-68.	Temperatures Contour Plot at 69 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-88
4-69.	Temperatures Contour Plot at 72 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions	4-89
4-70.	Temperature Versus Time During 84 Hour HCS Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-90
4-71.	Temperature Versus Time During Heatup Portion of HCS Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-91
4-72.	Temperature Versus Time During Cooldown Portion of HCS Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-92
4-73.	Temperatures Versus Time During the Last 24 Hours of HCS Process Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-93
4-74.	Temperature Contours at 3 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-94
4-75.	Temperature Contours at 6 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-95
4-76.	Temperature Contours at 9 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-96
4-77.	Temperature Contours at 12 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-97
4-78.	Temperature Contours at 18 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-98
4-79.	Temperature Contours at 24 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-99
4-80.	Temperature Contours at 30 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-100
4-81.	Temperature Contours at 36 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-101
4-82.	Temperature Contours at 42 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-102

4-83.	Temperature Contours at 48 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-103
4-84.	Temperature Contours at 54 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-104
4-85.	Temperature Contours at 60 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-105
4-86.	Temperature Contours at 63 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-106
4-87.	Temperature Contours at 66 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-107
4-88.	Temperature Contours at 69 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-108
4-89.	Temperature Contours at 72 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-109
4-90.	Temperature Contours at 75 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-110
4-91.	Temperature Contours at 79 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-111
4-92.	Temperature Contours at 81 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-112
4-93.	Temperature Contours at 84 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions	4-113

LIST OF TABLES

1-1.	Process Steps For the Hot Conditioning System	1-4
3-1.	N Reactor Fuel Dimensions	3-11
3-2.	Mole and Mass Fractions of Gases Found in the Standard Atmosphere .	3-17
4-1.	Flow Distribution in MCO with Mark Ia Baskets	4-2
4-2.	Flow Distribution in MCO with Mark IV Baskets	4-4
4-3.	Network and COBRA-TF Mass Flow Comparison	4-6
4-4.	Peak Fuel Temperatures for a Scrap Basket With Minimum Decay Heat, Minimum Porosity (0.259), and Helium Purge Gas	4-20a
4-5.	Derived Total Heat Transfer Coefficients from Scrap Basket HCS Process Simulation for Argon Purge, Nominal Decay Heat, and Porosity = 0.476	4-20a
4-6.	Derived Total Heat Transfer Coefficients from Scrap Basket HCS Process Simulation for Helium Purge, Nominal Decay Heat, and Porosity = 0.476	4-20b

APPENDICES

A.	FORTTRAN LISTING OF EFFECTIVE THERMAL CONDUCTIVITY PROGRAM	A-1
B.	FORTTRAN LISTING OF HYDRAULIC NETWORK PROGRAM	B-1
C.	CC:MAIL, T. D. COOPER TO F. J. HEARD, "HYDROGEN FROM HYDRIDE." . . .	C-1

Nomenclature
(SI and English Units)

Quantity	SI	English
Length	meter (m)	Inches (in.) or foot (ft)
Time (t)	second (s)	Second (s) or hour (hr)
Mass	Kilogram (Kg)	Pound (lbm)
Temperature (T)	Kelvin (K)	Fahrenheit ($^{\circ}\text{F}$) or Rankin ($^{\circ}\text{R}$)
Force (F)	Newton (N)	Pound (lbf)
Energy	Joules (J) or (N-m)	Btu
Gravitational Acceleration (a)	9.8066 m/s^2	32.1739 ft/s^2
Density (ρ)	kg/m^3	lbm/ft^3
Velocity (v)	m/s	ft/s
Pressure (P)	Pascal (N/m^2)	lbf/in^2
Dynamic Viscosity (μ)	Pascal-s (Kg/m-s)	lbm/ft-s
Kinematic Viscosity (ν)	m^2/s	ft^2/s
Specific Heat (Cp)	J/kg-K	Btu/lbm- $^{\circ}\text{F}$
Power	Watt (J/s)	Btu/hr
Heat Flux	$\text{J/m}^2\text{-s}$	$\text{Btu/ft}^2\text{-hr}$
Volumetric Heat Source	$\text{J/m}^3\text{-s}$	$\text{Btu/ft}^3\text{-hr}$
Heat Transfer Coefficient (h_c)	$\text{J/m}^2\text{-s-K}$	$\text{Btu/ft}^2\text{-hr-}^{\circ}\text{F}$
Thermal Conductivity (k)	J/m-s-K	$\text{Btu/ft-hr-}^{\circ}\text{F}$
Thermal Diffusivity	m^2/s	ft^2/s
Mass Diffusivity	m^2/s	ft^2/s
Volume Expansion Coefficient (β)	1/K	1/R
Surface Reaction Rate (mass units)	$\text{Kg/m}^2\text{-s}$	$\text{lbm/ft}^2\text{-s}$
Volumetric Reaction Rate (mass units)	$\text{Kg/m}^3\text{-s}$	$\text{lbm/ft}^3\text{-s}$
Heat of Reaction (mass units)	J/Kg	Btu/lbm
ρ_c	1 Kg-m/N-s^2	$32.174 \text{ lbm-ft/lbf-s}^2$
Stefan-Boltzman Constant (σ)	$5.6697\text{E-}8 \text{ J/s-m}^2\text{-K}^4$	$1.714\text{E-}9 \text{ Btu/hr-ft}^2\text{-R}^4$
Universal Gas Constant (R)	$8314.34 \text{ J/Kgmole-K}$	$1545 \text{ ft-lbm/lbm-mole}^{\circ}\text{F}$

1.0 INTRODUCTION

1.1 PURPOSE AND SCOPE

The purpose of this report is to document the results of a series of analyses that were performed to evaluate the thermal-hydraulic performance and feasibility of the proposed Hot Conditioning System (HCS) and process for the Spent Nuclear Fuel Project (SNFP). This completes the thermal-hydraulic assessment of the Integrated Process Strategy (IPS) that was begun in support of the Spent Nuclear Fuel Project (SNFP). Figure 1-1 presents the SNFP process flow showing the Hot Conditioning process step just prior of interim storage. The thermal-hydraulic evaluations that have been performed for the SNFP process flow steps prior to hot conditioning are documented within Heard 1996.

The subject efforts focus on investigating, quantifying, and establishing the governing heat production and removal mechanisms, flow distributions within, and performing simulations of the HCS and process operations for various configurations, obtaining preliminary results for comparison with and verification of other analyses, as well as, independently investigating each of the process steps, and providing technology based recommendations for consideration and incorporation into the design bases for the IPS.

The goal was to develop a series of thermal-hydraulic models that could respond to all process and safety related issues that may arise pertaining to the HCS. To this end the following deliverables have been proposed:

1. Determine the high temperature reaction rate relationships for uranium hydride decomposition and uranium metal oxidation
2. Develop a series of simple thermal models to evaluate the thermal performance of an MCO containing intact fuel, and/or fuel scrap (i.e., porous media) during the HCS passivation process
3. Develop a series of more detailed subchannel and/or finite-element coupled thermal-hydraulic models (including chemical reactions) to evaluate the internal MCO flow patterns and oxygen distribution for intact fuel assemblies during the HCS process
4. Develop a three-dimensional porous media model (including chemical reactions) to evaluate the thermal performance, internal flows patterns, and oxygen distribution for baskets consisting entirely of fuel scrap (i.e. rubble) through the entire HCS process.

These deliverables require that the appropriate thermal, hydraulic, and chemical reaction models be developed, verified, and used to perform the thermal-hydraulic assessment of the HCS. These efforts are also expected to provide clarification and identification of technical issues, as well as, provide the capability of performing parametric analyses for various fuel types, nuclear decay heat loads, degrees of fuel damage, and other variables such as thermal emissivities.

It is anticipated that the subject thermal-hydraulic models will form the basis for a series of advanced and more detailed models that will more accurately reflect the thermal performance of the IPS and alleviate the necessity for some of the more conservative assumptions and over simplifications, as well form the basis for the final process and safety analyses.

1.2 BACKGROUND AND OBJECTIVES

The SNF Project was established to develop engineered solutions to the expedited removal, stabilization, and storage of spent nuclear fuel and sludge from the K Basins at the U.S. Department of Energy's Hanford Site.

The SNF Project has an aggressive schedule to retrieve all fuel currently residing in the two K Basins (i.e, KW-105 and KE-105) and provide transport to the Canister Storage Building (CSB) for short/long term storage options. The retrieval efforts also include both removing the residual sludge from the fuel assemblies, basin floors and process pits, and disposal of the existing Fuel Encapsulation Canisters (FEC) and support racks.

The primary objectives of the subject model development and thermal-hydraulic analyses are as follows:

- Investigate, quantify, and establish the governing heat production and removal mechanisms and internal flow distributions for HCS operations.
- Evaluate each of the various HCS process steps for feasibility from an operational and safety viewpoint.
- Provide technology-based recommendations for consideration and incorporation into the design bases for the IPS processes.

A secondary objective is as follows:

- Independently review and assess results from other thermal analysts or outside consultants working on specific issues

1.3 HOT CONDITIONING SYSTEM AND PROCESS DESCRIPTION

After short term staging within the CSB, the Multi-Canister Overpack (MCO) containing up to 288 fuel assemblies is transferred by the MCO Handling Machine (MHM) to the hot vacuum conditioning station where the MCO is connected to the hot conditioning system. Hot conditioning consists of heating the MCO and fuel to approximately 300 °C (approximately 575 °F), which will remove the chemically bound water and decompose any uranium hydride producing uranium metal and hydrogen. The hydrogen is assumed to be released from the fuel and would be removed from the system or chemically react within the MCO with residual amounts of oxygen to produce water vapor, which would react with the uranium metal producing uranium oxide and more hydrogen gas until either the uranium hydride, the residual water vapor, or oxygen is depleted. A passivation step is then performed to reduce the overall chemical

reactivity of the small particles of uranium metal created by the decomposition of uranium hydride. The passivation step consists of cooling the MCO to approximately 150 °C and adding a controlled amount of oxygen to the MCO to oxidize a large fraction of the remaining highly reactive exposed uranium metal particles or surfaces. A time sequence for the HCS process steps is presented by Table 1-1 and Figure 1-2.

The hot conditioning process steps will proceed as follows: (1) MCO is received into the process cell by the CSB MHM; (2) the MCO within the process cell is connected to process gas piping, process off-gas piping, and process control systems; (3) the vacuum system is started to initiate flow through the MCO; (4) an inert gas is bled into the MCO and the vacuum pump continues to operate maintaining a purge flow through the MCO; (5) heating is started and the average MCO internal temperature is raised to 300 °C; (6) the MCO pressure in the MCO is reduced, and the MCO remains at an average temperature of 300 °C for an estimated 48 hours; (7) heating is reduced after 48 hours and a cooldown begins, gradually lowering the average temperature to 150 °C; (8) a slight partial pressure of oxygen is bled into the MCO using the inert purge gas as a carrier to passivate any remaining highly reactive surfaces; (9) the partial pressure of oxygen is gradually raised; (10) The MCO is maintained at 150 °C with sufficient oxygen present for passivation for approximately 12 hours; (11) heating is terminated and the MCO is allowed to cool to ambient; (12) the MCO is flushed with inert gas until no further oxygen is detectable within the MCO; (13) the MCO is isolated from and then disconnected from the process and off-gas systems; (14) the MCO is seal welded; (15) the top of the MCO is surveyed and decontaminated as necessary; and, (16) the MCO is removed from the process cell and placed in a long term CSB storage tube location (40 to 75 Years) by the MHM.

Table 1-1. Process Steps For the Hot Conditioning System.

- Load MCO into MHM, Transfer to Hot Vacuum Conditioning Process Station (8 hrs)
- Load MCO into Hot Vacuum Conditioning Process Station (4 hrs)
- Install Radiation Shield Into Place over MCO (4 hrs)
- Pre-Process Steps (8 hrs)
 - Initiate Cooling System
 - Place Process Hood onto MCO
 - Connect Process Lines
 - Seal Vent and Pressure Relief Ports (Install Seals and Blank Flange Covers)
 - Sample, Vent and Purge
- Remove Process Hood and Install Furnace Cover (4 hrs)
- Process Steps (96 hrs)
 - Purge with Inert Gas
 - Initiate Heatup to 300 °C at 12.5 °C/hr.
 - Achieve Vacuum, Hold for 48 Hours
 - Cooldown to 150 °C at 10 °C/hr.
 - Partial Oxidation with up to 20% O₂ Purge Gas, Hold for 12 Hours
 - Cooldown to Ambient at 10 °C/hr.
- Inert and Closure (24 hrs)
 - Remove Furnace Cover and Place Welding Hood onto MCO
 - Backfill with Inert gas
 - Disconnect Process Lines
 - Survey and Decontaminate
 - Weld Cover Plates at Process, Vent and Pressure Relief Ports and Inspect
 - Helium Leak Check MCO Process, Vent and Pressure Relief Ports
 - Survey and Decontaminate
 - Remove Weld Hood
- Remove MCO from Process Station with MHM (4 hrs)
- Transfer to CSB Support Tube (8 hrs)

Figure 1-1. Process Flow for the Spent Nuclear Fuel Project.

Figure 1-2. Process Times for the Hot Conditioning System.

2.0 SUMMARY

A series of analyses have been completed investigating the thermal-hydraulic performance and feasibility of the hot conditioning system (HCS) and process. The subject analyses used a series of one-, two-, and three-dimensional models that investigated chemical reactions, flow distributions, and combined thermal-hydraulic effects, including mass transport.

The subject analyses focus on quantifying the internal flow distributions within the multi-canister overpack (MCO), establishing the governing energy production and removal capabilities during the Hot Conditioning System (HCS) process steps, and performing process simulations for the various purge gases under consideration. The goal was to develop a series of thermal-hydraulic models that could respond to all process and safety related issues that may arise pertaining to the HCS, as well as obtain preliminary results for comparison with and verification of other analyses and provide technology-based recommendations for consideration by the HCS design authorities.

The results of the flow analyses indicate that the initial perforated base plate design for the Mark Ia and Mark IV fuel baskets resulted in either excessive bypass flow around the baskets or a maldistribution of flow around the fuel within a fuel basket. The optimum design would be zero bypass flow and a flow split of 59% to the inner flow channels and 41% to the outer most exterior surface of a given fuel assembly. The socketed base plate design does much better at obtaining the optimum flow splits, but still has approximately 14 to 21% bypass flow depending on the fuel type. The socketed base plate design is recommended for the Mark Ia and Mark IV fuel baskets.

The scrap basket, because of the high flow resistance associated with a porous media assumed similar to irregular shaped pieces of coal 0.75 inches in diameter, is predicted to have 46% bypass flow. With the addition of flexible flow restrictors, within the annulus between the scrap basket skirt and the MCO inner diameter, the bypass flow decreases to approximately 13 to 20% of the total MCO gas flow. Bypass flow restrictors are recommended for both the scrap and fuel baskets to maximize the amount of flow passing through the various baskets, during the passivation phase, to prevent the higher oxygen concentration in the bypass flow from obscuring the true oxygen concentration as measured by the process instrumentation.

Additional design work may be required to limit flow channeling through partially or unevenly filled fuel or scrap baskets. One possible design modification for consideration involves reducing the number and spacing of the flow holes through the scrap basket baseplate. This would result in the baseplate becoming the controlling resistance rather than the porous media and would minimize flow redistribution or flow channeling within a partially or unevenly filled scrap basket. The use of dummy fuel elements to completely load out a fuel basket may be a simple solution to effectively reduce flow channeling within a partially filled fuel basket.

Based on a series of one-dimensional parametric analyses, the length or amount of fuel that can be passivated by a given purge flow is a function of the temperature of the fuel, the concentration of oxygen within the purge gas,

and the amount of surface reaction area. The reaction length (the length required to consume all of the oxygen in the purge gas flow) decreases as the temperature of the fuel and reactive surface area increases. At a fixed surface temperature, the one-dimensional calculations indicated that reaction length will increase as O_2 concentration increases. While true for a constant axial temperature, this is misleading because the reaction rate is a function of both O_2 concentration and temperature. Therefore, in actual practice increasing O_2 concentration will increase the local reaction rate and hence the local surface temperature and will decrease reaction length. This expectation has since been confirmed through a series of three-dimensional analyses with variable oxygen concentrations by volume, which clearly show the reaction front starting at axial elevations with higher temperatures then moving down through the porous media or fuel baskets due to axial conduction and oxygen depletion. Axial conduction allows the near temperatures to increase just enough to react with oxygen and as the oxygen is depleted move toward the higher oxygen concentration (reduced reaction length). These findings are of course based on current understanding of the governing heat production and energy removal capabilities of the MCO within the HCS.

The following thermal results, conclusions, and recommendations are based on nominal chemical reaction rate relationships associated with unirradiated and uncorroded uranium metal with oxygen, a conservative estimate of the total reactive surface area of 800000 cm^2 for each scrap basket, and the conservative assumption that the upper six inches of each fuel assembly is completely de-clad. (NOTE: The above reactive surface areas are associated with the safety bases for the spent nuclear fuel project (SNFP)). The results of the thermal analyses indicate that careful consideration will need to be given to the location and variation of fuel temperatures within the MCO during the HCS passivation process to insure that:

1. Sufficient and a uniform distribution of oxygen reaches all exposed fuel surfaces such that highly reactive uranium metal is not left unpassivated in the MCO. This could occur if highly damaged fuel in the lower elevations of the MCO consume all the oxygen before it reaches the upper elevations of the MCO preventing fuel in the upper baskets from being passivated. This process may not be controllable for highly damaged fuel or scrap, since any reaction that starts will continue as oxygen continues to be added to the system or until all of the oxygen is consumed.
2. The chemical heat of reaction will be the dominate heat source at higher fuel temperatures and/or increased oxygen concentrations. This may lead to the fuel temperatures that could potentially exceed the alpha-beta phase change temperature leading to cladding failure and the extrusion of fuel into the flow channels, thereby increasing the reactive surface area many times and increasing the local reaction rate. Such a scenario may cause the fuel to melt during the passivation process step. An atmospheric ingress accident with 21% oxygen by volume will lead to a large energy spike and potentially excessive temperatures. A safety significant confinement system, a safety class confinement system, or an emergency inert gas blanketing system for the MCO, dewar flow annulus, and HCS vacuum chamber, depending on the results of a probabilistic safety analysis (PRA),

may be required to mitigate the consequences of an oxygen ingress accident and allow the chemical energy to slowly dissipate.

3. The high reaction heat, coupled with low heat removal capability, may also make the process hard to control. Hot spots within the MCO will be difficult to detect by the process instrumentation given the thermal time constant of the fuel, heat transfer to adjacent fuel assemblies or MCO structures, and the potential for significant oxygen bypass.
4. The presence of radial and axial temperature profiles in the fuel during passivation are likely to result in non-uniform oxygen consumption which will result in local hot spots in the fuel.

Other findings are summarized as follows:

1. The use of helium, rather than argon, as the HCS process purge gas can significantly reduce the heatup and cooldown times and is recommended as the purge gas of choice for the HCS process. Leakage and cost considerations may limit the effectiveness of this option. It is also recommended that a helium recycle system be investigated.

The proposed 12 hour HCS cooldown is not adequate for either argon or helium. Significant temperature gradients exist within the MCO, especially during the 12 hour HCS cooldown period prior to commencing the passivation phase. (Helium will minimize, but not completely eliminate temperature gradients.) These gradients could result in local temperatures sufficiently high enough to produce a chemically reactive hot spot given the oxygen feed during the passivation phase.

A minimum of a 12 hour extension beyond the 12 hour HCS cooldown period, while holding at an inlet temperature of 423.16 °F (302 °F), appears to provide an adequate time given helium as the purge gas to minimize the temperature gradients within the scrap basket prior to commencing the passivation phase. A hold time longer than 12 hours will be required for fuel baskets, given that the effective thermal resistance of the scrap basket is less than the fuel baskets, but has not yet been investigated. (Much longer hold times will be required for argon under any condition.) Any modification to the proposed HCS process times must be adequately investigated for thermal impacts on both the scrap and fuel baskets.

2. The presence of two scrap baskets (top and bottom) within an MCO leads to a set of unique thermal concerns. These are:
 - a. At the proposed inlet temperature of 150 °C (302 °F) the lower scrap basket will consume all the oxygen within the first few inches resulting in excessive temperatures (> 1000 °F). Reducing the inlet temperature by 50 °C allows oxygen to pass through the lower scrap basket to higher levels, but the increase in purge gas temperature as it reaches the upper scrap basket, produces the same temperature excursions as in the lower basket.

- b. A single chemically active "hot spot" within the scrap or fuel baskets will eventually lead to excessive temperatures. A "hot and cold spot" analysis given statistical variations in the decay heat, reactive surface areas, the geometrical area-to-volume ratio, and scrap basket local porosity has not yet been initiated.
 - c. Currently planned process instrumentation may not be able determine if the oxygen is being consumed on an distributed or localized "hot spot" basis. The purge gas flow from the MCO, as measured by the process instrumentation, could have a significant oxygen concentration due to bypass flow around the scrap and socketed fuel basket designs, while the remainder of the oxygen has been consumed in a very local area producing excessive fuel temperatures. It will be difficult to detect such local hot spots. As previously recommended, bypass flow should be minimized by using flow restrictors on both the scrap and fuel baskets. Other possible designs to minimize bypass flow include full length skirts that will intersect with each tier and a seal ring around the upper perimeter of the lower spider assembly.
 - d. The process instrumentation may not be adequate to detect the increase in purge gas temperature associated with a "hot spot", due to the long thermal time constant of the fuel or heat transfer to adjacent fuel and/or MCO internals.
 3. A single upper scrap basket is recommended.
 4. Given the potential variability in MCO contents, the HCS process operational strategies should be designed to allow for variable (0 - 5%) rather than a constant oxygen concentration and a variable helium purge gas flow rate (to be determined) that would help to minimize the radial and axial temperature gradients.
 5. The above conclusions and recommendations assume conservative reactive surface areas and published reaction rate relationships based on unirradiated and uncorroded uranium metal. Characterization data based on actual K Basin fuel is needed in these areas.

In summary, a uniform distribution of oxygen will be hard to achieve. Chemically active "hot spots" leading to excessive temperatures can occur via local variations in reactive surface area, temperature gradients, and oxygen concentrations. Additional model development and analyses are recommended to investigate combinations of scrap and fuel baskets within a MCO; such as, a less than the full complement of baskets, or a single upper or lower scrap and four fuel baskets, or five fuel and no scrap baskets. The following analyses are strongly recommended: (1) investigate the effects of decreased reactive surface areas, reaction rate relationships based on actual characterization data, variable process flow rates, a variable oxygen concentration feed during the passivation phase, and vacuum conditions, (2) investigate the effects of "statistical" based non-uniform distributions for decay heat, reactive surface areas, and scrap basket porosity, and (3) determine a modified HCS process heatup and/or cooldown rate, that could, respectively, in the minimum amount of time, obtain the minimum temperature necessary for complete dehydriding and

reduce the temperature gradients within the MCO prior to commencing the passivation phase. Items #1 and #2 must be performed to support the safety analysis report (SAR) and the final HCS design. (Item #2 is especially important when investigating the effects of chemically active "hot and cold spots" given a more realistic treatment of the variations expected with actual MCO loadings.) Item #3 must be performed to support HCS process operations given a final design or the assumed "statistical" variations in MCO loadings.

3.0 MODEL DEVELOPMENT, METHODOLOGY, AND ASSUMPTIONS

Temperature control involves maintaining an energy balance where the energy gains to the system equal the energy losses from the system. If the energy gains exceed the losses, the system temperatures will increase until the energy losses increase to balance the system. If the energy gains far exceed the capability of the system to reject energy, the temperature will continue to increase. The mechanisms for temperature control must be based on analytical studies that qualify the design and/or process operating limits necessary to prevent a temperature excursion.

The following sections discuss the current status of the thermal-hydraulic modeling efforts, the various computer programs that are being used to perform the HCS analyses and assessments, as well as the various technical issues associated with the thermal analyses.

3.1 STATUS OF THERMAL MODELING

One-, two- and three-dimensional finite-difference and finite-element thermal and thermal-hydraulic models of the HCS have been developed using the HUB¹ engineering spreadsheet, the COBRA-TF, and FIDAP² computer codes. [FIDAP has been validated and verified for use at Hanford (Heard 1994).] See Heard 1996 for a description of the HUB and FIDAP computer programs.

The COBRA-TF computer code was developed by the Pacific Northwest Laboratory for the United States Nuclear Regulatory Commission (NRC-1985) to perform analyses of thermal-hydraulic transients in various components of light water reactors. COBRA-TF is a three-dimensional finite difference model for two-phase, multi-species fluid flow and heat transfer. The code was originally developed for simulating single or two-phase flows within a variety of geometries associated with reactor components. The basic code is therefore suitable for modeling fluid flow and heat transfer within the MCO. Additional modifications have been made to the code to accommodate geometry and processes unique to the MCO passivation operation. These include an addition to the radiation sub-channel model to include the geometry of the fuel storage baskets, a revised heat transfer model for rubble in the scrap baskets and the addition of the specific hydride and oxidation reactions for uranium.

These models have been developed to perform an early evaluation of the thermal hydraulic technical issues associated with the HCS systems and proposed process. These models are considered sufficiently advanced to independently assess results from other thermal analysts, as well as provide clarification, identification and resolution of technical issues as they arise.

¹HUB is a registered trademark of Numerical Applications, Inc., Richland, Washington.

²FIDAP is a registered trademark of Fluid Dynamics International, Evanston, Illinois.

An inherent assumption in all of the earlier two-dimensional analyses is that by ignoring axial effects the resulting temperatures represent conservative values. It is anticipated that the subject sub-channel and three-dimensional models will more accurately reflect the thermal performance of the HCS and alleviate the necessity for some of the more conservative assumptions that existed in earlier analyses.

3.2 TECHNICAL ISSUES

The technical issues associated with the hot conditioning system include, but are not limited to, the following items: determining the supplied external heat necessary to achieve a given system heatup rate considering the various purge gases and decay heat loads, determining the purge gas flow rate to maintain a uniform internal MCO flow distribution, establishing adequate flow through the individual fuel assembly tiers, investigating the loss of convective flows under vacuum conditions, the effectiveness of purge gas flow for distributing oxygen throughout the system for the proposed passivation, determining the minimum time required at high temperatures to assure chemical decomposition of uranium hydride and/or passivation, the analysis of potential "cold" spots that would prevent local decomposition of uranium hydride, and/or "hot" spots that could locally consume all the oxygen feed and prevent passivation of other reactive fuel sites. Parametric analyses will be performed for many of the above issues including the effects of fuel type, decay heat load, and fuel damage.

Three of the above technical issues will effect thermal performance. They are: (1) fully defining the multiple and competing chemical reactions that will occur between water, water vapor, oxygen and uranium as a function of relative humidity, and oxygenated or oxygen free conditions, (2) determining the reaction surface area associated with corroded or breached fuel assemblies and the modeling of highly reactive "hot" or inactive "cold" spots, and (3) quantifying the rate at which the reacting mass (i.e. water vapor or oxygen) can be transferred to the reacting surface. This last issue involves assessing the effects of convective and diffusive mass transport as well as oxygen depletion within the MCO on the thermal performance of the MCO. Two secondary issues involve the uncertainties associated with various material properties. These are: (1) defining the effective thermal conductivity and viscosity for scrap basket given different purge gases and porosities, and (2) determining the emissivities of materials (including corroded fuel) as a function of surface condition and temperature.

All of the above issues must be thoroughly investigated and understood such that conditions within the MCO can be maintained to prevent chemical reactions from occurring to such an extent that a temperature excursion will occur, possibly compromising the mechanical integrity of the MCO during the HCS process.

The following sections discuss the issues associated with the chemical reactions rates and surface reaction areas, thermophysical properties, and mass transport.

3.2.1 Reaction Rates

The chemical reactions proceed at different rates depending on the individual reaction, activation energy, temperature of the fuel, the amount and form of reactant media involved; such as water, moist air, and for low pressure conditions the partial pressures of water vapor and the presence or not of oxygen. Readers are referred to Section 2.0 of Cooper 1996a, for a detailed discussion of the recommended reaction rates for unirradiated and uncorroded uranium metal and Section 3.4.1.2.3 of this report for a comparison of the Ritchie and Pearce rate relationships.

The rate of reaction of a particular reaction is usually presented in terms of milligrams (mg) of uranium (U), or oxygen (O₂) reacted per cm² per hour and is highly dependent on the surface area available for reactions, temperature of the fuel, and amount of reactants (i.e., water, water vapor or oxygen) to drive the reactions. The functional form of the above reactions are usually expressed in terms of a generalized Arrhenius Rate Law where the temperature dependence is usually treated as an exponential function and concentration dependence is usually treated via multiplication series and depends on the number of reacting species and order of the reaction. Reaction rate correlations remain to be developed for irradiated and corroded fuel. It is expected that a reaction rate relationship(s) will be developed from characterization data obtained by Pacific Northwest National Laboratory (PNNL) personnel using the data quality objectives (DQO) that have been developed for chemical kinetic studies of K West fuel samples (Lawrence 1995).

For multiple surface reactions the general form of the Arrhenius Rate Law remains, but subject to the rate at which mass can be transported to the reacting surface.

3.2.1.1 Chemical Reactions. For the HCS two chemical reactions are of interest. They are as follows:

The first reaction shows the decomposition and formation of uranium hydride in uranium metal and hydrogen gas. The first reaction can proceed both ways. The rate of hydriding and dehydriding is given by, Cooper 1996b, and depends on the equilibrium hydrogen pressure at a given temperature. This relationship is described further in Section 3.4.1.1.

The second reaction shows the reaction of uranium metal with oxygen to form uranium oxide. This reaction has been described by numerous authors (i.e., Ritchie and Pearce) and is discussed further in Section 3.4.1.2, where comparisons are made between the Ritchie and Pearce dry air reaction rate relationships. Additional discussion is provided in Section 3.4.1.2.4 with regard to a modified form of the Ritchie reaction rate relationship based on oxygen concentration.

3.2.1.2 Modeling of Hot and Cold Spots. The heat generation source term for chemical reactions is a function of the extent of fuel damage (i.e., reactive surface area), the temperature of the fuel, and the supply of water vapor

and/or oxygen to drive the reaction. For most conditions within a MCO, the reaction rate will be limited by the availability of reactants such as water vapor and oxygen to drive the reactions. The total heat generation source used in the subject analyses incorporates heat sources from both nuclear decay heat and chemical reactions.

The potential effects of degraded, badly damaged, or missing cladding on fuel on the thermal performance of the MCO have been accommodated within the various models and can be easily simulated by multiplying the chemical reaction rate for a given geometrical surface-to-volume ratio by a surface area enhancement (SAE) factor such as 0.5, 1, 2, 5, 10, etc. Multipliers greater than 1.0 simulate the effects of highly corroded fuel with a reactive surface area greater than the geometrical surface area. Multipliers less than 1.0 simulate reduced reactions that may be associated with fuel loss or oxide layers that might reduce the chemical reaction rate.

This methodology is appropriate for fuel elements and can be applied over the full or partial length of a given number of fuel elements or assemblies. However, the presence of a scrap basket containing pieces of fuel with an unknown amount of reactive surface area presents a unique problem.

The following methodology was used to obtain a conservative mechanism for determining the total chemical heat generation term within a given scrap (i.e., porous media) basket: (1) assume that the reacting basin surface area is $2.0 \times 10^6 \text{ cm}^2$ based on Cesium measurements, (2) assume that the fuel appears to be 10 times as reactive as the unirradiated uncorroded fuel used to generate the above area giving a reactive surface area of $2.0 \times 10^7 \text{ cm}^2$, (3) assume that the entire basin reacting surface is associated with scrap, and (4) assume that the entire volume of scrap is loaded into either 25 or 200 scrap baskets. The 25 scrap baskets result in 800000 cm^2 (80 M^2) per basket and defines the reactive surface area to be used as a safety bases. The 200 scrap baskets result in 100000 cm^2 (10 m^2) per basket and defines a more reasonable reactive surface area to be used with the process simulations. The reactive surface area is assumed to be evenly distributed throughout the scrap basket (i.e., porous media).

The nuclear decay heat values were derived from an inventory of the fuel stored in the K Basins (Willis 1995). The nominal and maximum values of 1.58 and 3.44 watts per fuel assembly were used to derive estimates of the nominal and maximum MCO heat generations rates of 426 and 929 watts per MCO, respectively. These estimates were derived for a loading of Mark IV fuel assemblies and are assumed to remain valid for the Mark Ia fuel assemblies. A minimum decay heat value of 0.53 watts per fuel assembly was derived assuming one-third of the nominal value. A MCO entirely comprised of minimum decay heat fuel assemblies would result in a total heat generation value of 142 watts per MCO. The maximum, nominal and minimum decay heat values of 929, 426, and 142 watts/MCO, correspond to volumetric heat rates of 2677, 1228, and 409 W/m^3 of fuel. For scrap basket thermal analyses, the volumetric heat rates must be adjusted by the assumed porosity, [(i.e., Decay Heat * (1 - POROSITY))].

The effect of "hot or cold spots" can be investigated as necessary within FIDAP or COBRA-TF by modifying the volumetric heat generation rate for a point or number of points. Hot and cold spots can also be modeled by changing the

thermo-physical properties of the elements that may be associated with degraded fuel or the absence of fuel. Thermo-physical property sets (i.e., density, specific heat, thermal conductivity, emissivity) representative of degraded or reacted fuel and/or cladding can be applied on an individual elemental basis. The absence of fuel can be modeled by changing the subject fuel elements to some other material, such as water, air or helium. Some iteration with the geometrical setup, subject to symmetry considerations, may be necessary to accommodate irregular shaped degraded fuel. The results of the "hot or cold spot" analyses will be provided at a later date as an addendum to this report.

3.2.2 Thermo-physical Properties, Effective Thermal Conductivity and Convective Heat Transfer Coefficients

All three modes of heat transfer were used: conductive, convective, and radiative. Radiative heat transfer is particularly noteworthy, since it involves a series of highly detailed but automated view-factor calculations involving a series of full or partially obstructing surfaces.

The thermophysical properties for density, specific heat, thermal conductivity, viscosities, and emissivities, as necessary, were obtained for the various materials from the SNFP Technical Databook (Short and Beary 1995). Currently, the following "solid" material properties are available for use; uranium metal (U), uranium oxide (UO₂), Zircaloy-4 (ZIRC), Aluminum (Al), stainless steel 304 (SS304), stainless steel 316 (SS316), and mild carbon steel (MCS). The following liquid and gaseous "fluid" material properties are available; water (H₂O), water vapor (VAPOR), air (AIR), Nitrogen (N₂), Oxygen (O₂), Helium (He), Argon (Ar), and Hydrogen (H₂).

Heat transfer through the heterogeneous porous media that makes up the rubble in the scrap baskets is calculated using a volume-averaged or effective thermal conductivity. The value of the total effective thermal conductivity (k_{eff}) used in the various models is determined from the sum of a molecular conduction component (k_g) and a thermal radiation component (k_r). The molecular conduction component uses Hadley's correlation which is a function of the porosity of the media and the thermal conductivity of each phase (uranium fuel and purge gas).

$$\frac{k_g}{k_r} = (1-\alpha_o) \frac{Pf_o + (k_g/k_r)(1-Pf_o)}{1-P(1-f_o) + (k_g/k_r)P(1-f_o)} \quad , \text{ where}$$

$$f_o = 0.8 + 0.1P \quad , \text{ and}$$

$$\log \alpha_o = -1.084 - 6.778(P - 0.298) \quad , \quad 0.298 \leq P \leq 0.580$$

$$\log \alpha_o = 0.405 - 3.154(P - 0.0827) \quad 0.0827 \leq P \leq 0.298$$

$$\log \alpha_o = -4.898P \quad 0 \leq P \leq 0.0827$$

Where P is the porosity, k_s is the solid phase conductivity and k_f the conductivity of the fluid phase. Based on the presentation given in Kaviany (1995) this correlation provides the best fit to the available test data for the range of parameters associated with the current analyses. The Hadley correlation does not however account for the effects of heat transfer by thermal radiation between particles within the porous media. Therefore, the radiant conductivity model of (Tien and Drolen 1987) as given in Kaviany (1995) was used to determine the radiation contribution k_r to the effective thermal conductivity.

$$k_r = 4 F d \sigma T_m^3$$

Where, the mean bed temperature T_m is given in terms of the emissive powers of the bounding black surfaces. The mean particle diameter is denoted by "d" and the radiative exchange factor by "F". An expression for the radiation exchange factor for particles with diffusive surfaces and porosities in the range from approximately 0.3 to 0.6 was obtained from Kaviany (1995).

$$F = 0.5756 \epsilon \arctan\left(\frac{C_s^{0.8011}}{\epsilon}\right) + 0.1843$$

$$C_s = \frac{k_s}{4 d \sigma T_m^3}$$

Where, ϵ is the particle surface emissivity and C_s is the adjusted effective solid thermal conductivity.

A FORTRAN program (Appendix A) was written to automate the calculation of the effective total thermal conductivity for uranium and three carrier gases; helium, nitrogen, and argon. The total effective thermal conductivity can be determined as a function of the porosity and temperature of the porous media.

Estimates of the convective heat transfer coefficients on the inside surfaces of the MCO for use with the COBRA-TF analyses were made using well known empirical treatments for free convection from vertical flat or cylindrical surfaces (McAdams 1954). Free or forced convection heat transfer coefficients for vertical plates or vertical cylindrical surfaces are some of the best known correlations and represent a small uncertainty to the energy balance. The assumption is that the MCO remain in a vertical position during the HCS process. FIDAP does not require convective heat transfer coefficients for solid surfaces adjacent to flow fields. The effective heat transfer coefficient due to conduction, convection, and radiation is explicitly calculated. A convective heat transfer coefficient is required for those surfaces (i.e., external) where the adjacent flow is not explicitly calculated.

Energy transfer between the interior surfaces and the MCO and between the MCO and the shipping cask or storage tube involve a combination of all three modes of heat transfer: conduction, convection, and radiation. At low pressures or for small gaps it is expected that convective heat transfer will be insignificant. Thermal radiation and conduction will remain. The thermal conductivity of gases and gas mixtures at low pressure conditions is not well

known and represents another source of uncertainty that may have an impact on the thermal performance of the proposed system during vacuum drying.

Radiative losses from the various surfaces depend on the surface area, the difference between adjacent surface temperatures to the fourth power, the view factor between the surfaces, and the emissivity of the surfaces. Emissivities for most materials as a function of temperature are rather sparse. Usually a single value at some temperature and surface condition (i.e., polished, pitted, oxidized, etc.) is quoted. The lack of emissivity data represents a significant uncertainty in the energy removal capabilities of the system. Emissivities provide an option for maximizing heat transfer by specifying that the subject surfaces be passivated or chemically treated to achieve high as possible emissivities. For radiative heat transfer from external surfaces, both the solar absorptivity and emissivity of the external surface, the ambient temperature, and solar heat flux must be specified.

3.2.3 Mass Transport

The three dimensional thermal-hydraulic models described in Sections 3.3, 3.4, and 3.5 model mass transport of the reacting species (i.e., water vapor, oxygen) to the reaction site. The chemical reaction rate affects the local volumetric heat generation and species concentration terms. The chemical reactions are now a function of the extent of fuel damage (i.e., reactive surface area), the temperature of the fuel, and the concentration of the reactants to drive the reaction. For most conditions within a MCO, the reaction rate will be limited by the availability and transport rate of the reactants.

The reaction rate and, hence, chemical energy will be especially important during the passivation portion of the HCS where scrap and/or fuel temperatures begin to rise as oxygen is transported through the system via a purge gas carrier. The chemical reaction is dependent on the local concentration of oxygen, which in turn is dependent on the rate of mass transport. The local chemical reaction rate will decrease as the amount of oxygen decreases.

3.3 FLOW DISTRIBUTION AND BASKET DESIGN

Hydraulic calculations have been performed to determine the expected flow paths through a loaded MCO during the hot conditioning and passivation process for several basket designs. These analyses consisted of investigating the gross flow splits within the MCO for fuel and scrap basket designs using a hydraulic network computer program. Additional analyses were performed with COBRA-TF to determine the individual sub-channel flows for an isothermal three-dimensional MCO model.

Knowledge of the flow distribution within an MCO is necessary as a basis for design and for operational decisions for the hot conditioning passivation process. Flow distributions can determine the degree of conditioning uniformity, the time required for passivation and the ability or accuracy by which the passivation process can be monitored. The following calculations evaluated several basket designs for Mark IA and Mark IV fuel elements. The

calculations all consider uniform loading of the MCO's with the exception of rubble in one of the Mark IV baskets. The calculations are considered scoping in nature because of the preliminary status of the basket designs and the relative simplicity of the hydraulic models.

3.3.1 Network Flow Distribution Models

The hydraulic modeling process consisted of first studying the MCO and fuel basket design drawings to determine the flow paths through the various components, then dividing these flow paths up into an equivalent hydraulic network of interconnected piping segments, determining the pressure loss across each segment based on empirical correlations, and finally using the conservation of mass to calculate the flow distribution through the equivalent hydraulic network. The solution procedure is iterative and a FORTRAN program (Appendix B) was written to perform this task. Details of the pressure losses and the solution technique for each of the basket designs discussed below is included as part of the documentation for Task Record PEA-96-007 and have been documented through a series of internal memos (Beaver 1996 and 1996a).

3.3.1.1 Mark IA Rerack Baskets. Two Mark IA rerack basket designs have been evaluated. The first, called the "perforated plate" design, is described on drawings H-2-826303 and is shown in Figure 3-1. The second, as shown in Figure 3-2, is called the "socket" design and was obtained from drawings SK-1-80208. For each of these designs the MCO was assumed to hold six baskets stacked end-on-end with 48 fuel elements in each basket for a total of 288 fuel assemblies per MCO. Dimensions for the Mark IA fuel elements were obtained from (Heard 1996) and are presented in Table 3-1.

As seen from Figure 3-1 the "perforated plate" type basket is essentially a thick walled annulus 22.5 inches high and closed at the bottom end with a perforated plate. The 8-inch diameter center cylinder contains a grapple adaptor and a 2-inch center bore to allow clearance for the draw tube which extends the length of the MCO from the base of the shield plug to approximately 1 inch from the bottom. The 48 fuel elements are placed on end in the basket. The bottom closure is perforated with 288 quarter-inch holes which allow space for water drainage and for gas flow during the hot vacuum conditioning and passivation process. With the fuel elements in place, it was estimated that only 132 of the holes in the bottom would remain unobstructed.

During the passivation process, an inert gas (assumed to be argon) containing a controlled amount of oxygen would be introduced into the MCO through the draw tube which exits at the bottom of the MCO. The gas would then flow radially outward through the bottom plenum and then either up through the perforations in the bottom basket or up between the outer wall of the basket and the inside wall of the MCO. In addition, some of the gas exiting the draw tube can flow back up through the annular space between the center bore in the baskets and the draw tube. This annular space is only partly sealed at the bottom of the MCO by a ring-shaped locator cone which fits between the draw tube and the center bore of the bottom basket. When stacked in the MCO, these type baskets form a seal which would prevent any gas

which flows up through the bottom perforations from communicating with the gas flow through the center annulus or between the baskets and MCO inside wall. An equivalent flow network for this basket design is shown on Figure 3-3. Note that the gas flow which passes through the open perforations at the bottom of each basket is directed either up through the interior of the 48 fuel elements or up around their outside surfaces. Since the baskets are slightly deeper than the fuel elements are long, the interior and exterior flows can mix prior to entering the base of the next basket in line.

The "socket" type design, as shown in Figure 3-2, places the fuel elements in individual sockets bored in the 3-inch thick baseplate. Fuel elements are retained in the sockets by a 1/4 inch wide bar welded across the bottom of each socket. The socket diameters are large enough to allow gas to flow either up through the interior of the fuel elements or around the outside. The outside wall for this basket design is a partial height perforated sheet which allows mixing of the gas which flows around the outside of the fuel elements with the bypass flow which passes between the base plate of the baskets and the MCO wall. When the baskets are stacked in the MCO the grapple adaptor on the center pipe is assumed to seal the area between the inside of the center pipe and the draw tube preventing mixing of the flow which bypasses around the locator cone at the bottom from mixing with the gas flow inside the baskets. The equivalent flow network used for this design is shown on Figure 3-4.

3.3.1.2 Mark IV Rerack Baskets. The two Mark IV fuel rerack basket configurations evaluated in this study were essentially the same design. The only differences were some clearances and details associated with the grapple adaptor and internals of the center tube. The "initial" design was obtained from drawing H-2-826303. Dimensions for the "prototype" design were obtained from drawing SK-2-300375. The basic construction for both designs is a center pipe surrounded by three concentric rings of wire mesh screen, all welded to a similar flat wire grating at the bottom. The baskets were assumed to contain 54 Mark IV fuel elements in each of five baskets for a total of 270 fuel assemblies per MCO. Dimensions for the Mark IV fuel were obtained from (Heard 1996) and are also presented in Table 3-1.

The basic Mark IV basket design is shown on Figure 3-5. The draw tube, bottom strainer and locator cone have the same configuration as those for the MARK Ia baskets. Gas flow exiting the draw tube will therefore pass radially outward through the bottom strainer before flowing up through the bottom grating of the baskets or between the basket and MCO wall. As with the Mark Ia design, some of the gas exiting the draw tube can flow back up through the annular space between the center hole in the baskets and the draw tube. Since the basket surfaces are all open mesh and since the fuel elements terminate below the base of the next basket in line, gas flowing through the interior of the fuel elements can mix with the gas flow past the exterior of the fuel elements which in turn can mix with the gas flow between the basket and MCO wall prior to entering the next basket. Gas flow between the draw tube and inside of the center pipe would not mix with the other flow paths because the grapple adapters form a basket-to-basket seal from the bottom of the MCO to the top. The equivalent flow network used for this design is shown on Figure 3-6.

3.3.1.3 Scrap Basket Hydraulic Model. As requested, the reference study (Beaver 1996) was extended to evaluate the flow distribution in a prototype SNF storage scrap basket during the hot conditioning and passivation process. It is possible that intact or partial Mark IV fuel elements could be placed on end (vertically) in the scrap basket prior to filling the remaining space within the basket with loose rubble. Since flow resistance associated with these fuel elements is less than that of the rubble surrounding them they constitute a path for bypassing flow around the rubble bed. This bypass flow would affect the passivation of the rubble and it could possibly be used as a gross means for controlling the passivation process within the rubble.

The current calculations have evaluated the amount of bypass flow as a function of the number of intact or partial fuel elements placed in the scrap basket along with the rubble. The calculations also investigated the effect a proposed seal between the outside surface of the scrap basket and the MCO wall would have on the amount of flow bypassing the rubble.

The hydraulic network model described in Section 3.3.1.2 was modified to simulate the latest scrap basket design. Included in this scrap basket simulation is a hydraulic model for a combination of rubble and intact or partial fuel elements. The model also contains the proposed seal between the side wall of the basket and inside wall of the MCO.

The scrap basket design evaluated in these calculations is described on drawings SK-1-80209 and shown in Figure 3-7. The basket design is essentially a thin walled cylinder 22.625 inches in diameter and 26.85 inches long. It is closed at one end with a 1/4 inch plate which is perforated with 1 inch diameter holes which are covered with wire cloth having 4 meshes per inch. A 2-5/8 inch diameter pipe at the center of the basket contains the grapple adaptor and provides attachment for the radial divider plates which separate the basket contents into 6 sectors. The flexible seal attached to the side wall of the basket was assumed to have 1/16 inch wide slots at 2 inch intervals around the periphery of the basket.

The calculations assumed that various intact or partial Mark IV fuel elements could be placed on end (vertically) in the scrap basket prior to filling the remaining space within the basket with loose rubble. Since flow resistance associated with these fuel elements is less than that of the rubble surrounding them they constitute a path for bypassing flow around the rubble bed. The amount of flow bypassed would depend on the rubble configuration, and the number, configuration and condition of the fuel elements placed in the rubble basket.

For purposes of this evaluation the rubble within the basket was modeled as a bed of loose (randomly packed) irregular shaped particles with a mean diameter of 3/4 inch. Porosity of the rubble was assumed to be 0.46, which is equivalent to measurements for hard coal with a similar mean diameter. Height of the rubble in the basket was 25 inches. Fuel elements were assumed to be undamaged. Partial elements were assumed to be full length sections of only the outer cylinder.

Table 3-1. N Reactor Fuel Dimensions.

Fuel Type	Mark-IA	Mark-IV
Overall Nominal Dimensions (inches)		
Outer element OD	2.404	2.425
Outer element ID	1.767	1.701
Inner element OD	1.246	1.279
Inner element ID	0.440	0.479
Cladding Thickness (mils)		
Outer element, outer clad	25	25
Outer element, inner clad	25	20
Inner element, outer clad	40	30
Inner element, inner clad	25	20
Nominal Maximum Length (inches)		
Outer element	20.88	26.10
Inner element	20.82	26.04
Assumed End Cap Thickness (inches)		
Outer element	0.200	0.200
Inner element	0.200	0.200

3.3.2 Three-Dimensional MCO Flow Model

A detailed three-dimensional iso-thermal flow model of the MCO internals was constructed using the COBRA-TF thermal/hydraulic simulation code. The model was prepared in order to verify proposed design and operating conditions for the hot vacuum conditioning and passivation process. Details of the model are described below.

For purposes of design evaluation the MCO was assumed to contain a total of five storage baskets loaded axially end-to-end. Of the five baskets, two are assumed to contain scrap, one placed at the top of the MCO and the other at the bottom. The remaining three fuel storage baskets at the center of the MCO are assumed to contain 54 intact Mark IV fuel elements each. Depth of the rubblized fuel in the scrap baskets was taken to be 25 inches. The assumed MCO axial configuration is shown on Figure 3-8 and a cross section of the scrap and fuel storage baskets are shown on Figure 3-7. The MCO configuration and dimensions were obtained from drawing SK-2-300379, details for the fuel storage baskets from SK-1-80208 and the scrap baskets from SK-1-80209.

The COBRA-TF model divides the MCO into 7 vertical sections. Starting at the bottom of the MCO these include an inlet plenum, a rubble basket, three

fuel baskets, a rubble basket and an outlet plenum (See Figure 3-9). Because of symmetry about the centerline only a 30° segment of the MCO is modeled explicitly. Each section is divided into a number of vertical and lateral flow channels that are defined by the section geometry. Figure 3-10 illustrates the vertical flow channels assigned to a fuel basket containing Mark IV fuel assemblies. The lateral flow channels for this same section are shown on Figure 3-11. Note that lateral flow between channels internal to the fuel elements and those external to the fuel elements takes place only in the region between the top of the fuel elements and the bottom of the next basket.

The vertical channels within each section are further divided into a series of axial nodes that provide the locations at which the momentum and energy equations are solved (see Figure 3-9). For analysis of the hot conditioning operation, purge gas is introduced from the draw tube at the center of the inlet plenum at a specified rate. The purge gas is then allowed to flow upward through the MCO where it exits the outlet plenum through the discharge channel in the MCO shield plug. Flow distribution within the MCO is calculated based on the friction and momentum loss between nodes. Friction loss is calculated by the code based on the wetted surface areas and the fluid Reynolds number. Momentum loss between nodes is calculated based on loss coefficients input to the code. The loss coefficients are based on empirical correlations for the various types of geometry.

The inlet plenum is treated as a free volume with pressure loss for the lateral flow through the inlet strainer, along the MCO base plate and the spacer bars. The inlet plenum also provides connection to the vertical flow channels through the scrap basket, between the scrap basket and MCO wall and between the draw tube and the storage basket center pipe.

The scrap basket is treated as a porous media rubble bed and represents a modification to COBRA-TF. Pressure loss across the rubble bed is calculated using an empirical correlation (Idelchik 1986) which is a function of the height of the bed, the mean particle size, the bed porosity and the fluid temperature rise across the bed. The current calculations assume that the rubblized fuel in the scrap basket has a mean diameter of 0.75 in., a porosity of 0.46 and a bed height of 25 inches (similar to a basket of hard coal). The hydraulic model for the scrap basket also includes loss coefficients for the perforated bottom plate and for an assumed flexible seal between the outside wall of the scrap basket and inside wall of the MCO.

The "socket" type design for the fuel storage baskets allows the purge gas entering the basket from below to flow directly through the interior channels of each fuel element. The design also includes two paths which bypass flow around the outside of the fuel elements. The first path is next to the fuel elements and is produced by the clearance between the outside diameter of each fuel element and the inside diameter of the base plate socket. The second bypass channel is around the outside surface of the storage basket through the clearance between the basket and inside wall of the MCO. This passage could potentially prevent oxygen in the purge gas from reacting with the uranium metal on the surface of the fuel elements during the passivation process. However, since the outside skirt on the basket is perforated and only partial height (11 inches) the bypass flow can mix with the gas flowing past the outside surface of the fuel elements and potentially with the interior gas flows in the space between the top of the fuel elements

and bottom of the next storage basket. Fluid friction losses for flow through and around the fuel storage baskets is calculated within COBRA-TF based on the input geometry and the fluid Reynolds number. Momentum losses are calculated based on loss coefficients input to the code. The loss coefficients are based on empirical correlations for the various types of geometry (Idelchik 1986).

Temperature dependent material properties for the uranium metal (fuel), zircalloy cladding, and 304 stainless steel (storage baskets and MCO) were obtained from (Short and Beary 1995). Thermophysical properties for either the argon or helium hot passivation purge gas were also obtained from the SNFP Technical Databook. Thermal conductivity of rubble in the scrap baskets was calculated using a correlation based on the ratio of the thermal conductivity of the solid phase (uranium) to that of the fluid phase (argon or helium) and the assumed porosity. The particular correlation used is described in Section 3.2.2.

Details of the COBRA-TF input for both the thermal and hydraulics calculations are included in the analysis task record (PEA-96-11) which may be made available upon request.

3.4 MCO PASSIVATION MODELS

A series of parametric thermal-hydraulic analyses were performed using the HUB engineering spreadsheet program to evaluate the passivation phase of the hot vacuum conditioning (HVC) process. The subject analyses evaluated the length of fuel within a multi-canister overpak (MCO) necessary to support a given reaction rate as a function of fuel temperature, fuel damage (or more specifically, surface reaction area), and oxygen content. Additional studies evaluating the dehydriding phase using a recently obtained reaction rate relationship (Appendix C) for the decomposition of uranium hydride (UH_3) are currently being incorporated into the various thermal models.

3.4.1 One-Dimensional Scoping Models

Hot conditioning requires that sufficient oxygen be supplied to all of the reactive fuel surfaces such that each surface may be sufficiently oxidized to passivate the fuel against further oxidation reactions during longer term storage. This work was initiated to assure that fuel having varying degrees of fuel damage and varying amounts of hydride can be adequately treated during the passivation phase of hot conditioning.

This will require that: (1) a sufficient amount of oxygen be introduced into the inert gas to passivate the fuel, and (2) that the oxygen be reasonably uniformly distributed to all of the reacting surfaces within the MCO. This requires temperature control of the fuel surfaces such that highly damaged fuel surfaces will not consume all of the available oxygen in the MCO, preventing oxygen from reaching all surfaces and not passivating these surfaces within the time period allowed for hot conditioning.

This also requires that the thermal-hydraulic and chemical reaction analyses be performed to quantify the parameters for hot conditioning such that the end objectives can be satisfied. The initial effort toward this end

has been to perform scoping studies that will provide first order estimates for the flow splits through the MCO (Section 3.3) and the reaction rates (Section 3.4) that can be anticipated given known quantities for fuel reaction surface area.

The spent nuclear fuel that is currently stored in the K basins will eventually be removed from the basin, dried in a cold vacuum drying facility and temporarily stored in the Canister Storage Building (CSB). The fuel will be stored in Multi-Canister Overpak containers (MCO) that will hold five or six baskets of fuel containing 48 or 54 fuel elements, depending on the type of fuel being stored, i.e., Mark IA or Mark IV fuel.

After short term staging within the Canister Storage Building (CSB), the MCO is transferred by the MCO Handling Machine (MHM) to the hot vacuum conditioning station where the MCO is connected to the hot vacuum conditioning system.

Hot conditioning consists of two steps: (1) the dehydriding phase and (2) the passivation phase. During the first phase the fuel is heated to 300 °C. The uranium hydride is decomposed and the chemically bound water is released. Hydrogen gas is released during the hydride decomposition reaction that takes place at this temperature, and fresh uranium is left exposed at the reaction surface. The hydrogen gas will be carried out of the MCO with the inert gas that is being passed through the system. The dehydriding phase of the HCS was not explicitly analyzed in time for inclusion within this report. It is anticipated that the results of this effort will be supplied at a later date as an addendum to this report.

The second phase, passivation, will then be carried out to oxidize this fresh uranium. This process will be carried out at a temperature near 150 °C. Oxygen gas will be introduced into the inert gas at a predetermined rate to react with the uranium, reducing the uranium's capacity to further react with water or oxygen during interim storage.

The following paragraphs describe the reaction rate relationships that were used for the dehydriding and passivation portions of the HCS process.

3.4.1.1 Hydride Reaction Rate Relationship. A model for calculating the rate of uranium hydriding and dehydriding is given by Cooper 1996 (Appendix C) as follows;

$$\alpha = a \cdot \ln(P_0/P) \cdot \exp(-E/RT) \cdot \Delta t \quad (3-1)$$

where, α = Normalized extent of the reaction for any assumed amount of initial hydride
 a = 92.8333 sec⁻¹
 P = Hydrogen partial pressure (Pa)
 P_0 = Equilibrium hydrogen pressure (Pa) = 133.3*10^(A/T+B)
 E/R = (18900 cal/gmmole)/(8314.34 J/Kg mole-°K) or 9517.81 °K
 T = Fuel temperature (°K)
 Δt = Time interval (sec)

where, for hydriding ($P_o > P$)

$$A = 3473 \text{ } ^\circ\text{K}$$

$$B = 8.05$$

and, for dehydriding ($P_o < P$)

$$A = 4717 \text{ } ^\circ\text{K}$$

$$B = 9.46$$

For the dehydriding process, the extent of the reaction is equal to the fraction of hydride mass present at time zero that has decomposed over the time interval Δt and for the hydriding process it is equal to the fraction of available uranium that can be hydrided. There are three moles of hydrogen gas formed for every two moles of UH_3 decomposed.

It is assumed that the partial pressure of hydrogen in Equation (3-1) is constant. This will not be the case in a sealed MCO, since for the dehydriding process, the hydrogen concentration will continuously increase until it reaches the equilibrium concentration. The hydrogen concentration will decrease for the hydriding process until the equilibrium concentration is reached. The equilibrium concentration will be continually changing since it is a function of the fuel temperature, which changes during the various process stages due to the changing ambient conditions.

3.4.1.2 Dry Air Reaction Rate Relationships. The recommended reaction rate relationships for unirradiated and uncorroded uranium in dry air are given by Cooper 1996a. The reaction rates given by Cooper, as described by Ritchie 1981 and Pearce 1989, are compared in the following sections. The actual reactions will occur in the presence of an inerting gas, probably helium or argon, into which oxygen has been introduced at a predetermined level, probably on the order of 0% to 5% by volume.

3.4.1.2.1 Ritchie Relationship. The Ritchie equation for the reaction of uranium in dry air is given below. The reaction rate in terms of Kg of $\text{U}/\text{m}^2\text{-s}$:

$$RR = K \cdot \text{EXP}(-E/RT) = 1916.67 \text{EXP}(-9215.67/T) \quad (3-2)$$

where,

RR = Reaction rate of uranium in dry air ($\text{KgU}/\text{M}^2\text{-s}$)

K = Reaction rate constant, $6.9\text{E}+8 \text{ mgU}/\text{cm}^2\text{-hr}$ or
 $1916.67 \text{ KgU}/\text{M}^2\text{-s}$

E = Activation energy, $18300 \text{ cal}/\text{gmMoleU}$ or
 $7.6622\text{E}+7 \text{ J}/\text{KgMoleU}$

R = Universal gas constant, $1.98575 \text{ cal}/\text{gmMoleU-}^\circ\text{K}$ or
 $8314.34 \text{ J}/\text{KgMoleU-}^\circ\text{K}$

T = Temperature ($^\circ\text{K}$)

The reaction rate constant from Equation 3-2 can be written in terms of Kg of oxygen; where, the reaction rate constant of $1916.67 \text{ KgU}/\text{M}^2\text{-s}$ is equivalent to $257.7 \text{ KgO}_2/\text{M}^2\text{-s}$

The time required to react uranium to a given depth can be calculated from the following equation

$$RD = \frac{\rho \cdot D}{RR \cdot C} \quad (3-3)$$

where, RD = Time to react (hr) to given depth
 D = Reaction depth (M)
 ρ = Density of uranium, 18822 KgU/M³
 RR = Reaction rate from EQU (3-2) KgU/M²-s or kgO₂/M²-s
 C = Conversion constant, 3600 s/hr

As an example using Equations 3-2 and 3-3, the time (hr) required to react uranium to a depth of 2mm (0.002m) at a constant temperature of 200 °C (473.16 °K) is approximately 1569 hours.

The heat of reaction per Kg of uranium is assumed

$$\Delta H_U = 259.3 \text{ kcal/gmMoleU} = 4.564 \text{E}+6 \text{ J/KgU}$$

The same heat of reaction in terms of oxygen is assumed

$$\Delta H_{O_2} = 3.395 \text{E}+7 \text{ J/KgO}_2.$$

3.4.1.2.2 Pearce Relationship. The Pearce equations for the reaction of uranium in dry air are given below. The equation is written for two temperature ranges.

$$\text{Log } K = 8.9464 - 4638.2/T \quad (T < 597^\circ\text{K}) \quad (3-4)$$

$$\text{Log } K = 28.381 - 7 \log T - 4638.2/T \quad (T > 597^\circ\text{K}) \quad (3-5)$$

where, K = Reaction rate (mgO₂/cm²-hr)
 T = Temperature (°K).

The Pearce equation can be rewritten to obtain a reaction rate relationship based on KgO₂/M²-s as follows

$$RR = 2.7778 \text{E}-6 \cdot 10^{\text{Log } K} \quad (3-6)$$

where, RR = Reaction rate of uranium in dry air (KgO₂/M²-s) given K from either Equation 3-4 or 3-5 depending on the temperature.

3.4.1.2.3 Comparisons of Ritchie and Pearce Reaction Rate Relationships. Figure 3-12 compares the Ritchie reaction rate relationship for the oxidation of uranium in dry air with the Pearce reaction rate relationship for the oxidation of uranium in dry air. Both relationships are plotted as a function of temperature. The Ritchie equation predicts a higher reaction rate for all temperatures. The Pearce reaction rate relationship clearly shows a change in the reaction rate at 597 °K, which corresponds to the temperature intervals for Equations 3-4 and 3-5.

3.4.1.2.4 Modified Ritchie Reaction Rate Relationship for Variable Oxygen Concentration. The reaction rate constant, K, in Equation 3-2 was derived for the oxygen concentration in the standard atmosphere. Table 3-2 presents the mole and mass fractions of the various gases found in the standard atmosphere. The mass fraction of oxygen in the standard atmosphere is 0.23143.

Table 3-2. Mole and Mass Fractions of Gases Found in the Standard Atmosphere.

Species	Mole fraction	Mass fraction
Nitrogen (N ₂)	0.780840	0.75520
Oxygen (O ₂)	0.209476	0.23143
Argon (A)	0.009340	0.01288
Carbon dioxide (CO ₂)	0.000314	0.00048
Neon (Ne)	0.000018	0.00001
Helium (He)	0.000005	0.00000
Totals	0.999993	1.00000

Equation 3-2 is assumed to be based on data taken from tests in which an unlimited supply of fresh air with a constant oxygen concentration is available. Equation 3-2 is not valid for a gas mixture with changing O₂ concentration or other mixtures different from air.

However, since no other information is currently available, we make the assumption that Equation 3-2 is a function of the molar concentration of oxygen in the gas mixture and that this effect is contained in the reaction rate constant. Hence, to remove this effect, K, must be divided by the concentration of O₂ in air

$$K' = \frac{K}{[C_{O_2}]^n} = \frac{K}{\left[\frac{MF_{O_2}^{AIR}}{MW_{O_2}} \cdot \rho_{AIR} \right]^n} \quad (3-7)$$

where,

- K = Reaction rate constant = 1916.67 kgU/m²-s or 257.7 kgO₂/m²-s
- [C_{O₂}] = Molar concentration of O₂ in air (kgmoleO₂/m³)
- n = Order of reaction = 0.77 (see Section 3.5.1.2.5)
- MF_{O₂}^{AIR} = Mass fraction of O₂ in std. atmosphere = 0.23143 (kgO₂/kgAir)
- MW_{O₂} = Molecular weight of O₂ = 31.999 (kgO₂/kgmole O₂)
- ρ_{AIR} = density of air (kgAir/m³) for a given P (Pa) and T (°K).

where, ρ_{AIR} = PMW_{AIR}/RT.

Since the general Arrhenius Reaction Rate relationship can be written as

$$R = Ae^{(-E/RT)} C_A^a C_B^b \dots C_N^n$$

where, A can be replaced with K' from above.

Therefore, for the $U+O_2 = UO_2$ reaction where the mass fraction of uranium is assumed to remain equal to 1, Equation 3-2 can be modified as follows

$$RR = \frac{K}{\left[\frac{MF_{O_2}^{AIR}}{MW_{O_2}} \cdot \rho_{AIR} \right]^n} \cdot e^{(-E/RT)} \cdot \left[\frac{MF_{O_2}^{MIX}}{MW_{O_2}} \cdot \rho_{MIX} \right]^n$$

Simplifying,

$$RR = K' e^{(E/RT)} \cdot \frac{(MF_{O_2}^{MIX} \rho_{MIX})^n}{(MF_{O_2}^{AIR} \rho_{AIR})^n}$$

$$RR = K' e^{(-E/RT)} \cdot \frac{(MF_{O_2}^{MIX} MW_{MIX})^n}{(MF_{O_2}^{AIR} MW_{AIR})^n} = K' e^{(-E/RT)} \left(\frac{MF_{O_2}^{MIX} MW_{MIX}}{MF_{O_2}^{AIR} MW_{AIR}} \right)^n \quad (3-9)$$

where, for a two species mixture

$$VF_{O_2} = \text{volume fraction of } O_2 = \frac{V_{O_2}}{V_{TOTAL}} = \frac{P_{O_2}}{P_{TOTAL}} = \frac{\# \text{ moles } O_2}{\# \text{ moles Total}}$$

$$MF_{O_2}^{MIX} = \text{mass fraction of } O_2 \text{ for a mixture} = \frac{VF_{O_2}^{MIX} MW_{O_2}}{VF_{O_2}^{MIX} MW_{O_2} + (1 - VF_{O_2}^{MIX}) MW_{CARRIER}} \left(\frac{kg_{O_2}}{kg_{MIX}} \right)$$

$$\frac{1}{MW_{MIX}} = \sum_{i=1}^2 \left(\frac{MF_i}{MW_i} \right)$$

$$MF_{O_2}^{AIR} = 0.23143 \left(\frac{kg_{O_2}}{kg_{AIR}} \right)$$

$$MW_{AIR} = 28.97 \left(\frac{kg_{AIR}}{kg \text{ mole AIR}} \right)$$

The reaction rate for any concentration of oxygen in air or any other carrier gas can now be determined. An inherent assumption to Equation 3-9 is that the carrier gas has no effect on the reaction rate. Furthermore, the same volume concentration of oxygen in different carrier gases give identical reaction rates.

For example, assume 2% O₂ by volume in helium and 2% O₂ by volume in argon;

$$\begin{aligned}
 K &= 257.7 \text{ kgO}_2/\text{m}^2\text{-s} \\
 e^{(-E/RT)} &= e^{(-9215.67/T)} \\
 MW_{AIR} &= 28.97 \left(\frac{\text{kg Air}}{\text{kgmoleAir}} \right) \\
 MW_{He} &= 4.003 \left(\frac{\text{kgHe}}{\text{kgmoleHe}} \right) \\
 MW_{Ar} &= 39.948 \left(\frac{\text{kgAr}}{\text{kgmoleAr}} \right) \\
 MF_{O_2}^{AIR} &= 0.23143 \left(\frac{\text{kgO}_2}{\text{kgAir}} \right) \\
 MF_{2\%O_2}^{He+O_2} &= 0.140257 \left(\frac{\text{kgO}_2}{\text{kgMIX}} \right) \\
 MF_{2\%O_2}^{Ar+O_2} &= 0.0160843 \left(\frac{\text{kgO}_2}{\text{kgMIX}} \right) \\
 MW_{MIX}^{He+2\%O_2} &= 4.56292 \left(\frac{\text{kgMIX}}{\text{kgmoleMIX}} \right) \\
 MW_{MIX}^{Ar+2\%O_2} &= 39.78902 \left(\frac{\text{kgMIX}}{\text{kgmoleMIX}} \right)
 \end{aligned}$$

The reaction rates (KgO₂/m²-s) can now be determined.

Helium

$$RR = K \cdot e^{(-E/RT)} \cdot \frac{(0.140257 \times 4.56294)^n}{(0.23143 \times 28.97)^n} = K e^{(-E/RT)} \times 0.095455^n$$

Argon

$$RR = K \cdot e^{(-E/RT)} \cdot \frac{(0.0160843 \times 39.78902)^n}{(0.23143 \times 28.97)^n} = K e^{(-E/RT)} \times 0.095455^n$$

By comparison, both the reaction rates for 2% O₂ in helium and argon are identical. The modified Ritchie reaction rate relationship gives the same reaction rate for variable oxygen concentrations regardless of the carrier or purge gas, where n was determined to be 0.77 as discussed in Section 3.4.1.2.5.

3.4.1.2.5 Regression Fit to Available Oxygen Data. A limited amount of reaction rate data for both variable temperatures and oxygen concentrations was summarized by Ritchie (1981), but never reduced to a reaction rate relationship. This data was recently regressed for variable oxygen concentrations in dry air. This data covers a temperature range of 423.16 °K (302 °F) to 673.16 °K (392 °F) and an oxygen pressure from 800 Pa (0.116 psi) to 31990 Pa (4.641 psi). The functional form is as follows;

$$RR = \frac{3.7339E-7 P_{O_2} / 1kPa}{(A3 \cdot T - A2) T + A1 + (P_{O_2} / 1kPa) ((B3 \cdot T - B2) \cdot T + 131)} \quad (3-10)$$

where,

- RR = Reaction rate (kgO₂/m²-s)
- P_{O₂} = Oxygen pressure (kPa)
- A₁ = 1220.6008677
- A₂ = 5.0432385 (1/°K)
- A₃ = 0.0052256 (1/°K²)
- B₁ = 318.58388066
- B₂ = 1.34663517
- B₃ = 0.001423998

Comparison of Equation 3-9 with Equation 3-10 suggests that the reaction rate exponent, n, should have a value of 0.77. This comparison is illustrated in Figures 3-13a through Figures 3-13g, where the modified Ritchie Rate Relationship (n = 0.77) (EQU 3-9) is compared to regressed Ritchie data (EQU 3-10) for volume fractions ranging from 1% to 21% oxygen. Very good agreement is obtained for a modified Ritchie exponent of 0.77. Figure 3-14 presents the reaction rate resulting from the modified Ritchie Rate Relationship (n = 0.77) in dry air versus temperatures for a series of different oxygen volume fractions.

3.4.1.3 Reaction Lengths. The length of fuel required to completely react all of the oxygen in the flow as a function of fuel temperature, T, O₂ partial pressure, P, fuel reaction area per unit length, A, and the total gas volumetric flow rate, Q, is given by the following expression;

$$RL = \frac{P \cdot Q \cdot MW}{A \cdot RR \cdot R \cdot T} \quad (3-11)$$

- where, RL = Reaction length (M)
- P = Partial pressure of oxygen (Pa) or (N/M²)
- Q = Volumetric flow rate (M³/s)
- MW = Molecular weight of oxygen (31.999 KgO₂/KgMoleO₂)
- A = Fuel surface reaction area per unit length of fuel
- = 25.353 M²/M = 25.353M (assuming 54 fuel elements in a basket)
- RR = Reaction rate (Kg/M²-s) from EQUATION (3-9)
- R = Universal gas constant 8314.34 J/KgMoleO₂-°K
- T = Temperature (°K)

and, 1N = 1Kg-M/s² and 1J = 1N-M.

The heat generation rate per unit length of fuel (J/M-s) is given by the following expression assuming an unlimited supply of oxygen;

$$HL = \Delta H_{O_2} \cdot A \cdot RR_{O_2} \quad (3-12)$$

where, HL = Heat generation rate per unit length of fuel (J/M-s)

ΔH_{O_2} = Heat of reaction, $3.395E+7$ J/KgO₂,

A = Fuel surface reaction area per unit length (M)

RR_{O₂} = Reaction rate in terms of oxygen (KgO₂/M₂-s)

The heat generation rate (J/s) due to the complete reaction in a given flow can be determined by the following expression

$$H = \Delta H_{O_2} \cdot \left(\frac{P \cdot Q \cdot MW}{R \cdot T} \right) \quad (3-13)$$

where, H = Heat generation rate (J/s)

ΔH_{O_2} = $3.395E+7$ J/KgO₂

P = Partial pressure of oxygen (Pa) or N/M²)

Q = Flow rate (M/s)

MW = Molecular weight (31.999 KgO₂/KgMoleO₂)

R = Universal gas constant (8314.34 J/KgMoleO₂-°K)

T = Temperature (°K).

3.4.2 Three-Dimensional Integrated MCO Model

The integrated thermal-hydraulic COBRA-TF model of the MCO for hot conditioning and passivation evaluations utilizes the flow model described in Section 3.3.2, but also includes two sources of heat as input to the fuel elements and uranium metal scrap and a third source due to the HCS process operation. The first heat source is radiolytic decay and the second is chemical related to oxidation of the fuel. The third heat source is that produced by operation of the hot passivation station and is applied to the outside wall of the MCO and treated as an input boundary condition to the model.

The radiolytic decay heat used in the analyses assumes a total of 929 watts for an MCO containing 270 Mark IV fuel elements (0.0446 W/in³ of fuel). For the model of intact fuel elements this value is volume weighted over the inner and outer fuel annuli. For the scrap basket model this value is applied to the non-porous volume of the scrap. With a porosity of 0.46 the resulting decay heat input to the scrap basket is very similar to that of a 54 element fuel storage basket. Chemical energy due to the reaction between uranium metal and oxygen was also included in the analyses. The reaction rate relationship that was used is based on a modified form of the Ritchie reaction rate relationship based on oxygen concentration. See Section 3.4.1.2.4 for additional discussion.

Heat transfer between the fuel, the purge gas and the inside walls of the surrounding MCO is calculated within the code as a combination of convection, conduction, and thermal radiation. Heat transfer coefficients for convective flows are calculated by the code as a function of the local Reynolds number, wetted perimeter of the flow passages and thermophysical properties of the purge gas. In the limit, as flow goes to zero, the convective heat transfer becomes simple heat conduction. Convective heat transfer within the scrap basket rubble bed is calculated similar to that for the intact fuel elements except that the heat transfer area is determined from the fuel volume and an estimated surface to volume ratio associated with the assumed porosity of the rubble.

Radiant heat transfer is determined between surface nodes at the same axial location. Radiation in the axial direction is neglected because of geometry effects (axial view factors are generally small) and because axial temperature gradients are also generally small. The radiating surfaces within the model are assumed to be grey and the intervening gas transparent and non-participating. Emissivity is input for each surface as a function of the material type. Surface view factors are calculated by the code based on subchannel templates (geometry surrounding a particular flow channel). Additional templates were added to the code to accommodate the "socket" type fuel storage baskets. Radiation heat transfer within the rubble bed itself was treated as part of the effective thermal conductivity (see Section 3.2.2). Radiation heat transfer between the outside surface of the scrap basket and inside wall of the MCO is included in the model.

3.5 MCO HOT CONDITIONING MODEL

3.5.1 Three-Dimensional Detailed Single Tier Models

Two, detailed three-dimensional models of a fuel basket and a scrap basket within a MCO within the HCS station were constructed using the FIDAP thermal-hydraulic simulation code. Each of the thermal-hydraulic models were developed to investigate the range of temperatures and heat up rates associated with each of the proposed HCS process for both the scrap basket and fuel tiers that could be present within an MCO as well as provide validation of the HUB and COBRA-TF models previously discussed in Sections 3.4.1 and 3.4.2. Computer limitations prevented the development of a full length finite-element three-dimensional model of a MCO.

For the purposes of simulation, the MCO was assumed to contain a total of five storage baskets loaded axially end-to-end and was in place within the HCS station. Two of the five baskets were assumed to contain scrap, while the remaining three baskets are assumed to contain intact Mark-IV fuel assemblies. Figures 3-15 and 3-16 present the conceptual design of the Hot Conditioning System.

The subject 3-D models considered one scrap tier and fuel tier. Figures 3-17 through 3-20 present the two fundamental geometries that were utilized to construct the fuel and scrap basket tier models. Figures 3-17 and 3-19 present planar cross sectional views of the two geometries; whereas,

Figures 3-18 and 3-20 present isometric three-dimensional views of the two geometries. The two fundamental geometries consist of the following:

- A three-dimensional 30-degree sector model of a single fuel basket or tier containing the equivalent of 54 Mark IV fuel assemblies within a MCO positioned within the HCS station.
- A three-dimensional 30-degree sector model of a fully loaded single scrap basket or tier within a MCO positioned within the HCS station.

The above FIDAP models assumed that the inlet flow and temperature distributions to each tier are known and supplied as input. These can be estimated based on hand calculations, simple HUB calculations, or COBRA-TF calculations.

For the correct treatment of thermal radiation within three-dimensional domains, the radiating surfaces must be fully enclosed. For the small gaps associated with the basket skirt-MCO ID and MCO OD - Jacket ID, this enclosure is provided by two vertical surfaces, the two reflective surfaces associated with the lines of symmetry, and the upper and lower planes associated with the inlet and outlet flow boundaries. The first four surfaces are automatically handled within FIDAP, however, for "windows" and "openings", e.g., an inlet or outlet flow boundary, a reference temperature for calculating the radiative heat transfer must be supplied as a boundary condition by the user.

For the inlet flow boundary, this is fairly simple. A uniform inlet temperature and flow distribution can be assumed. The outlet temperature, especially with chemical reactions, is more difficult to estimate, thus requiring an iterative approach where T_{REF} is updated based on the mean outlet temperature from the previous run. This treatment usually requires a single iteration to obtain agreement within five degrees of the mixed mean outlet temperature and the assumed T_{REF} . A slight conservatism is imposed such that T_{REF} is always slightly greater than the mixed mean temperature.

3.5.1.1 Fuel Basket. A single fuel basket thermal-hydraulic model was developed from Figures 3-17 and 3-19. This model is an extrusion of an earlier two-dimensional thermal model that was documented in Heard 1996. A representative nodalization pattern for the fuel tier is presented by Figure 3-21.

In most cases the model definition data, material property sets and simulation control information remain identical from one model to another, only the geometry differs. Table 3-1 presents the N Reactor Mark IV fuel dimensions that were used for the three-dimensional fuel model. The overall axial length of the Mark IV fuel elements range from 17.4 to a maximum of 26.1 inches. The overall axial length of the Mark Ia fuel elements range from 14.3 to a maximum of 20.9 inches. The three-dimensional fuel tier model assumed Mark IV fuel with a uniform length of 26.1 inches.

The MCO outer diameter was assumed to be 24 inches with a wall thickness of 0.5 inches. A 1.0 inch diametrical gap was assumed between the MCO outer diameter and the HCS heating jacket (or dewar) inner diameter. The HCS jacket

outer diameter was assumed to be 26 inches with a wall thickness of 1.0 inches.

Energy gains and losses from the system involve heat transfer from the inner fuel elements to the outer surface of the MCO via conductive, convective, and radiative heat transfer mechanisms. Clearly the correct treatment of the energy gains and system boundary loss mechanisms is very important. For the subject models all three modes (i.e., conduction, convective, and radiative) of heat transfer were incorporated via specialized surface or continuum elements. Internal to the model conductive, convection, and radiative heat transfer was allowed. Energy was removed from the system by convection and radiative heat transfer only.

Convective heat transfer was allowed. Energy was removed from the MCO and HCS via the forced air flow jacket heating and cooling system. Convective losses from the inner surface of the MCO and scrap basket skirt occurred due to forced flow through the scrap/rubble (i.e., porous media) from the separate HCS gas processing system. Convective heat transfer coefficients are explicitly calculated by FIDAP and need not be applied for any interior surface adjacent to a flow field. FIDAP does require that a convective heat transfer coefficient be entered to account for convective losses where a flow field is not calculated, such as the external surface to the system. The jacket OD was considered to be an adiabatic (zero heat flux) surface. No losses from the jacket OD were allowed.

Radiative heat transfer is particularly noteworthy, since it involves a series of highly detailed automated view-factor calculations performed by FIDAP involving a series of full or partially obstructing surfaces within the interior of the scrap tier model. The view factors were calculated on an individual element basis for all elements comprising radiative surfaces. Radiative heat transfer has been found to be very significant, especially under vacuum conditions when natural circulation is not possible and the thermal conductivity of gases is reduced. A grey body approach without participating media was assumed for each of the radiating surfaces within the model. The outer surface of the system was assumed to be an adiabatic surface with no energy losses from conductive, convective, or radiative heat transfer.

Solar insolation was not considered. Only nuclear decay heat and chemical reactions were modeled as energy sources.

The geometry for this model is complete, but the input necessary to describe the problem has not yet been established. This model was put on hold in favor of developing a full length integrated MCO COBRA-TF model. If necessary, the above tier model can be completed to investigate specific issues within a given tier using inlet and outlet conditions supplied by COBRA-TF.

3.5.1.2 Scrap Basket. A porous rubble bed thermal-hydraulic model was developed from Figures 3-18 and 3-20. A representative nodalization pattern for a scrap basket tier model is shown in Figure 3-22. The porous rubble bed thermal-hydraulic model requires both fluid and solid properties. The amount of solid and fluid material are related via the porosity of the porous media. The solid properties are assumed to be those of uranium metal, but can be changed to uranium oxide or any other material mix as desired. The fluid

properties are assumed to be mixes of various gases such as oxygen, water vapor, hydrogen, argon, etc. For the finite elements within the porous entity the volume averaged porous media momentum, continuity, species, and energy equations are solved.

The rubble bed or scrap model was developed assuming a Mark IV fuel basket was completely filled with scrap to a depth of 26.1 inches. The lower baseplate was assumed covered with a fine screen mesh able to retain rubble with diameters greater than 0.25 inches. The scrap basket inlet velocity was derived from the mass flow rate determined from the hydraulic network models discussed in Section 3.3 assuming an inlet temperature of 423.10 °K. The hydraulic network assumed a MCO volumetric inlet flow rate of 10 scfm (14.7 psi, 60 °F).

The HCS jacket heating/cooling mass flow rate was based on 250 scfm at 14.7 psi at 423.16 °K. The corresponding flow velocity was based on a 1.0 inch diametrical gap which was assumed between the MCO outer diameter and the HCS jacket inner diameter.

For a porous entity, a flow model must also be defined. The Darcy momentum equation was specified via user input. A bulk permeability $1.0\text{E-}7\text{m}^2$ equivalent to a matrix of beryl saddles and large irregular bumps (Kavinay 1995) was also specified. The bulk fluid viscosity was set equal to that of the carrier or purge gas; either helium, nitrogen, or argon depending on the calculation.

The effective heat capacity of the porous entity is determined by the following equation

$$\langle \rho C_{p,eff} \rangle = \rho_f C_{p,f} \phi + (1-\phi) \rho_s C_{p,s} \quad (3-14)$$

where, ρ_f , $C_{p,f}$, ρ_s , and $C_{p,s}$ refer to the density and specific heat of the fluid (f) and solid(s) phases, respectively and ϕ refers to the porosity of the porous media.

The effective thermal conductivity of a porous media as currently employed by FIDAP is determined by the following simple equation based on parallel conduction

$$K_{eff} = K_f \phi + (1-\phi) K_s. \quad (3-15)$$

This equation tends to maximize the effective thermal conductivity and is not appropriate for metallic matrixes filled with gases. However, the thermal conductivity corresponding to the fluid and solid phases can be transformed to reflect values necessary to derive a total K_{eff} based on other correlations.

For example, the particular correlation that was used for determining the effective thermal conductivity was Hadley's, which is referenced in Kavinay (1995) and discussed in Section 3.2.2. Hadley's correlation appears to match the available conductivity data for packed particle beds in the range

of porosities from 0 to 0.58 with the ratio of $K_{\text{solid}}/K_{\text{fluid}}$ corresponding to the range associated with a metallic matrix filled with liquids or gases. Readers are referred to Kavinay (1995) for a complete discussion of effective thermal conductivities for heterogenous porous media.

Hadley's correlation returns a value based on the ratio of effective thermal conductivity divided by the thermal conductivity of the fluid phase at a given temperature and porosity

$$K_{\text{eff}}/K_f = A.$$

Solving for K_f yields the transformed thermal conductivity for the fluid phase as input $K_f = AK_{\text{eff}}$.

Substituting into the Equation 3-15 and solving for K_s yields the transformed thermal as input for the solid phase;

$$K_s = K_{\text{eff}} - AK_{\text{eff}} \phi / (1 - \phi).$$

Substituting both transformed variables K_f and K_s into EQU 3-15 yields

$$K_{\text{eff}} = K_{\text{eff}}$$

Figure 3-23 compares the effective thermal conductivities versus temperature based on Hadley's correlation for a uranium metal matrix with helium, nitrogen, and argon carrier gases for the porosities of 0.259 and 0.476. These values can be compared to the thermal conductivity of uranium metal, which ranges from approximately 26.8 (100 °K) to 39.1 (1040 °K) J/m-s-°K.

3.5.2 Three-Dimensional MCO Simple Ring Model

A simplified COBRA-TF model of the MCO within a shipping cask or a hot conditioning station jacket was developed from the detailed model previously discussed in Section 3.3.2 and 3.4.2.

The simplified COBRA-TF model was developed to perform fast running simulations where the thermal response times are on the order of several days and where complex 3-D models would require a large amount of computer resources and are not capable of fast running simulations.

The complex three-dimensional thermal radiation capability in COBRA-TF was modified so that, as an option, a simple two-dimensional radial and axial approach could be used. The modified radial radiation capability plus the radial/axial conduction model was used to analyze a test case to demonstrate and validate this fast running simulation capability.

The model consists of seven equivalent volume preserved metal rings as shown in Figures 3-24 and 3-25. Metal ring 1 is the inner support tube, rings 2-5 are the fuel, ring 6 is the basket shroud, and ring 7 is the MCO. Although the cask, ring 8 is shown here, for this simulation it is not included since a water bath at constant temperature is assumed, which would keep the cask at constant temperature so it is not necessary that the cask be

modeled in this case. Ring 8 would also serve to provide bounding conditions for simulating the hot conditioning system. The model also includes 7 equivalent volume preserved gas rings, gas rings 1-7. Ring 8, shown in the figures is not included explicitly in the model, but is treated as a constant temperature boundary condition. Five vertical baskets of fuel are included in this particular simulation, however, since all are treated uniformly there are no axial temperature gradients computed in this simulation.

The inner support tube, basket shroud, and MCO are stainless steel with an emissivity of 0.25. The fuel is treated as being all uranium, but with an exterior surface emissivity of 0.40 representative of zircaloy cladding. The equivalent rings of fuel preserve the volume of the outer and inner fuel elements combined, and the exterior surface of the outer fuel element, but do include the interior surfaces. Other analysis has shown that the interior element is generally only a few degrees different in temperature than the exterior element and therefore thermal transport between the exterior and interior element does not need to be simulated. Both volume and interior and exterior surface areas of the support tube, basket shroud, and MCO are preserved. In this simulation, the basket shroud is assumed to be without perforation holes and to extend the full length of the fuel. The radiation view factors across each gas gap in this simulation from the interior surface to the exterior surface are assumed to be 1.0.

For this simulation the gas volume external to the fuel elements is preserved, however, the gas volume internal to the fuel elements is not. This volume can be included if a particular simulation such as vacuum drying depressurization or MCO pressurization is being conducted.

The MCO once drained of liquid will contain only residual water, inert gas, or steam during normal process and storage operations. During accident conditions it could contain air. The inert fill gas for this simulation is assumed to be argon.

The test case simulated a MCO surrounded by a 50 °F water bath with fuel assemblies and an inert gas, Argon. The 50 °F water bath supplied a boundary condition appropriate for the cold vacuum drying system. The above boundary condition can be changed to 302 °F (150 °C) to simulate the hot conditioning system. The simulation was initiated with the MCO and contents at 50 °C at atmospheric pressure and sealed. A heatup transient was simulated for several days to arrive at a steady-state condition. The steady-state results are compared to a steady state analytical solution for thermal radiation and conduction between a series of vertical plates.

The results of the model validation are shown in Figure 3-26 where the analytical solution and the COBRA-TF solution at near steady state are compared.

Prior analysis has demonstrated that only certain heat transport phenomena dominate most spent nuclear fuel thermal response situations that must be simulated. These include radial thermal radiation, radial and axial conduction, radial and axial convection of gas and liquids, evaporation of liquid or phase change of water to steam. These dominant transport phenomena can be treated by adding a simple radial thermal radiation capability to COBRA-TF. Simulation capability of this new capability in COBRA-TF has now

been demonstrated and validated. A computer tool is now available capable of simulating all the dominant phenomena, with reduced man-hours for development of model input, and significant reductions in computer run time. The modified COBRA-TF model was used to simulate the heatup transient associated with the HCS. The results of this simulation are presented in Section 4.4.

Figure 3-1. Perforated Plate Basket Design for Mark Ia Fuel.

Figure 3-2. Socket Basket Design for Mark Ia Fuel.

Figure 3-3. Hydraulic Network for Perforated Plate Type Fuel Baskets.

0071C

Figure 3-4. Hydraulic Network for Socket Type Fuel Baskets.

00718

Figure 3-5. Wire Mesh Basket Design for Mark IV Fuel.

Figure 3-6. Hydraulic Network for Wire Mesh Type Fuel Baskets.

Figure 3-7. Cross Section View of Scrap and Mark IV Fuel Assembly Baskets.

Figure 3-8. MCO Configuration for Integrated Model.

Figure 3-9. COBRA-TF Model of MCO.

Figure 3-10. Vertical Flow Channels for Fuel Assembly Storage Basket.

Figure 3-11. Lateral Channels for Fuel Assembly Storage Basket.

Figure 3-12. Comparison of the Ritchie and Pearce Reaction Rate Relationships in Dry Air versus Temperature.

Figure 3-13a. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 21% Oxygen by Volume in Dry Air.

Figure 3-13b. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 10% Oxygen by Volume in Dry Air.

Figure 3-13c. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 5% Oxygen by Volume in Dry Air.

Figure 3-13d. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 4% Oxygen by Volume in Dry Air.

Figure 3-13e. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 3% Oxygen by Volume in Dry Air.

Figure 3-13f. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 2% Oxygen by Volume in Dry Air.

Figure 3-13g. Comparison of Modified Ritchie Reaction Rates Relationship with Regressed Data for 1% Oxygen by Volume in Dry Air.

Figure 3-14. Reaction Rate in Dry Air versus Temperature for Different O_2 Volume Fractions.

Figure 3-15. Conceptual Design of Hot Conditioning System Containing a MCO Shown Without Shield Plug and HCS Upper Components.

4061E

Figure 3-16. Representative Flow Patterns for Lower Scrap Basket Within MCO at the HCS Station.

Figure 3-17. Planar View of the 30° Sector Model of a MCO Tier Containing Mark IV Fuel Assemblies Within the HCS.

Figure 3-18. Planar View of the 30° Sector Model of a MCO Tier Containing Scrap Fuel Within the HCS.

Figure 3-19. Three-Dimensional Isometric View of a 30° Sector Model of a MCO Tier Containing Mark IV Fuel Assemblies Within the HCS.

Figure 3-20. Three-Dimensional Isometric View of a 30° Sector Model of a MCO Tier Containing Scrap Fuel Within the HCS.

Figure 3-21. Nodalization Pattern for Three-Dimensional Fuel Basket Tier Model.

Figure 3-22. Nodalization Pattern for Three-Dimensional Scrap Basket Tier Model.

Figure 3-23. Effective Thermal Conductivity Based on Hadley's Correlation for Uranium Metal and Various Carrier Gases for Porosities of 0.259 and 0.476.

TempleGraph 2.5, Origin: -94453@ucag1 - Mon Jul 15 11:53:45 1996 (data file was keff.dat)

Figure 3-24. Ring Model for Simplified Three-Dimensional MCO COBRA-TF Model.

Figure 3-25. Blow Up of Ring Model for Simplified Three-Dimensional MCO COBRA-TF Model.

Figure 3-26. Comparison of Radial Temperature Gradient From Simplified COBRA-TF Model versus Analytical Solution.

4.0 RESULTS

Section 4.0 presents the results from series of analyses that were performed using the COBRA-TF, HUB, and FIDAP computer codes to assess the Hot Conditioning System and proposed process, as illustrated by Figure 1-2.

The models discussed in Section 3.0 and the results as presented within this section are judged to have satisfied the deliverables presented in Section 1.1

4.1 FLOW DISTRIBUTION VERSUS BASKET DESIGN

4.1.1 Mark IA Baskets

Flow distribution through an MCO with the "perforated plate" basket design is shown in Table 4-1. As indicated by the first column in the table, 80% of the total gas flow is predicted to bypass the fuel elements in the baskets. It is calculated that 74% of the gas would flow between the outer wall of the baskets and the inside wall of the MCO and 6% of the total flow would bypass through the annulus between the draw tube and center hole of the baskets. Because almost all of the pressure loss associated with flow through the basket occurs in the 1/4 inch holes in the bottom plate the flow split between interior and exterior surfaces of the fuel elements is essentially governed by the ratio of the number of holes open to the interior of the fuel elements to those open to the space exterior to the fuel elements. The assumed hole distribution gives 11% of the total flow through the interior of fuel elements and 9% past the exterior.

Because of the large bypass flow between the baskets and MCO wall, a modification to the basic "perforated plate" design was also evaluated. For this case, a seal ring was assumed to be added to the ends of the six radial spacer bars, which form the plenum between the base plate of the bottom basket and the bottom of the MCO. Since this seal ring would eliminate any communication between the bottom plenum and the annular space between the basket and MCO side walls, six 1/8-inch slots were assumed to be cut in the seal ring to allow any water trapped between the baskets and MCO wall to drain into the lower plenum. Gas flow distribution for this configuration is included in the second column on Table 4-1. A comparison of the flow split without and with the seal ring indicates that the basket/MCO wall bypass flow has been reduced from 74% to 3% of the total passivation flow. The 3% represents the gas flow through the six slots in the seal ring. The increased pressure drop across the MCO increases the bypass flow between the draw tube and basket center hole from 6% to 20% but also increases the flow past the fuel elements from 20% to 77%. Again, the flow split between flow passages within the fuel elements and between fuel elements is governed by the assumed distribution of holes in the basket base plate.

The last two flow split comparisons shown on Table 4-1 are for the "socket" type design. For the basic design the total flow bypassing the fuel elements is estimated to be 13%, which is the smallest for the two configurations evaluated. Also, since the basket sidewalls are essentially

non-existent, the 11% of total flow which bypasses between the base plate of the basket and MCO side wall is free to mix with the gas flow which passes between the side walls of the sockets and exterior surface of the fuel elements. As indicated in the table, 87% of the total flow is predicted to pass directly by the fuel elements with 59% flowing through the interiors and 28% around the exterior.

Other design constraints may require the clearance between the base plate of the basket and inside MCO wall to increase over what has been evaluated. An increase in the base plate/MCO clearance could adversely affect the fuel element internal/external flow split. Therefore, results of a modification to the base plate design which adds a flexible seal to this bypass area are presented in the final column in Table 4-1. For this case, the flow bypassing the fuel elements is reduced to only 3% of the total. The predicted flow split for the fuel is 66% through the interior and 31% past the exterior. Note that the surface area for the fuel elements is distributed 59% interior and 41% exterior, which is reasonably well matched by the flow split predicted for the socket-type basket design. This matching of flow splits and fuel surface area is important if uniform passivation of the fuel elements is to be achieved.

Table 4-1. Flow Distribution in MCO with Mark Ia Baskets.

Flow Channel	Perforated Plate Design	Perforated Plate (mod.) ⁽¹⁾	Socket Design	Socket Design (mod.) ⁽²⁾
Basket/MCO wall bypass	74	3	11	0
Draw tube/basket center	6	20	2	3
Fuel elements (interior @ 59% of total surface area)	11	41	59	66
Fuel elements (exterior @ 41% of total surface area)	9	36	28	31

Note: The flow values are given in percent of total flow through the MCO.

⁽¹⁾ A seal ring which blocks the flow area into the MCO wall bypass annulus was added to the design.

⁽²⁾ A seal ring which blocks the flow area between the basket baseplate and MCO wall, was added to the design.

4.1.2 Mark IV Baskets

Flow distribution within an MCO with the Mark IV rerack basket designs is listed in Table 4-2. The first column in this table presents the calculated flow distribution for the "initial" Mark IV basket design. This design has the opposite characteristics from those of the "perforated plate" design for the Mark Ia fuel in that the pressure loss through the bottom

grating of the basket is small in comparison with that through the interior of the fuel elements. Therefore, predictions show that 75% of the total flow into the MCO would flow around the exterior of the fuel elements and only 9% would flow through the interior channels. The 13% flow which is estimated to flow between the outside of the basket and MCO wall is free to mix with the flow around the exterior of the fuel elements because of the large flow area through the wire mesh side walls of the basket. Only 3% of the flow is predicted to bypass between the center pipe and draw tube.

Making the basket side walls solid and adding a seal ring to the bottom of the MCO, similar to the modification described for the Mark Ia basket design, does little to improve the flow distribution through the MCO. This is indicated by the calculations presented in column 2 of Table 4-2. While the basket/MCO side wall bypass flow is reduced to nearly zero, the flow split through the fuel elements is not improved. Again, this poor flow split results from the fuel elements being the primary pressure loss and that the flow area around the outside of the fuel elements is significantly greater than that through the interior.

The predicted flow distribution for the "prototype" design is presented in column 3 of Table 4-2. The results are essentially the same as the "initial" design since the most significant design changes are associated with the center tube and have very little effect on the MCO hydraulics.

Placing rubble in the baskets was expected to have a significant affect on the MCO flow distribution. Therefore, a preliminary investigation was made by assuming that the inner and middle ring of the bottom MCO basket contained rubble to a depth of 25 inches and a mean diameter of 3/4 inches. The outer ring was assumed to contain 23 MARK IV fuel elements. Results of the calculations are indicated in column 4 of Table 4-2. The large difference in flow resistance between the rubble and intact fuel elements causes the gas flow to bypass the rubble in favor of the fuel elements in ring 3 (78% of the total) and the area between the basket and MCO wall (17%). Only 2% of the total flow is predicted to pass through the rubble. Gas flow through the draw tube/basket center bypass or through the remaining baskets in the MCO is not affected by the presents of rubble in the bottom basket.

The effect of filling the entire bottom basket with rubble is shown in column 5 of Table 4-2. For this configuration 11% of the total gas flow is predicted to flow through the rubble. The remaining 89% bypasses the basket either around the outside next to the MCO wall or up the center of the basket adjacent to the draw tube.

For comparison purposes, the final column in Table 4-2 presents the flow splits anticipated for a Mark IV "socket" design identical to the Mark Ia "socket" design discussed earlier, except that the number of fuel assemblies has been increased from 48 to 54. The Mark IV flow splits for this design concept are very similar to the Mark Ia splits presented in Table 4-1. As indicated in Table 4-2, 47% (16% bypass + 31% exterior flow) of the total flow is free to mix between the bypass channels and the outermost exterior surface of the fuel assemblies with 50% flow through the interior flow channels. The remaining 3% bypasses the baskets by flow up the center pipe and around the draw tube. This closely matches the actual distribution of surface area; 41% exterior to 59% internal surface area.

From the standpoint of fuel passivation these results indicate that the mesh type basket design for Mark IV fuel does not lend itself well to providing a flow split past the fuel elements which approximates the ratio of surface areas requiring passivation. The proposed "socket" design achieves a flow split much closer to the actual surface areas important if uniform passivation of the fuel elements is to be achieved. Furthermore, if rubble is to be placed in the MCOs with other intact fuel elements, it is not clear from the flow distribution results alone how or where it should be placed. Some criteria must be developed that defines what fraction of the total fuel complement must be passivated and what time limits will be placed on the process. Given a set of criteria, the hydraulic calculations should then be coupled with thermal/chemical reaction calculations to determine the best rubble loading option(s).

Table 4-2. Flow Distribution in MCO with Mark IV Baskets.

Flow Channel	Initial Design	Initial (mod) ⁽¹⁾	Prototype Design	Prototype w/rubble ⁽²⁾	Prototype w/rubble ⁽³⁾	Socket Design ⁽⁴⁾
Basket/MCO wall bypass	13	.2	12	17	84	16
Draw tube/basket center	3	4	3	3	5	3
Fuel elements (interior @ 59% total surface area)	9	11	7	5 (ring 3)	--	50
Fuel elements (exterior @ 41% total surface area)	75	85	78	73 (ring 3)	--	31
Rubble	-	-	-	2	11	--

Note: The flow values are given in percent of total flow through the MCO.

- (1) Outside surface of the baskets assumed to be solid and a seal ring added at the entrance to the MCO wall bypass area.
- (2) Rubble is assumed to be placed in the inner two rings of the bottom basket. The outer ring 3 is assumed to contain 23 fuel elements.
- (3) The entire bottom basket is assumed to contain rubble.
- (4) Identical to Mark Ia design; except 54 fuel elements.

4.1.3 Scrap Basket

The percentage of MCO passivation flow which bypasses the rubble in the scrap basket as a function of the number fuel elements contained in the scrap basket is presented on Figures 4-1 and 4-2. Figure 4-1 presents the calculated results for intact (complete) fuel elements and Figure 4-2 similar results for partial fuel assemblies outer elements only. Each figure presents the calculations with and without the seal between the basket side wall and inside wall of the MCO.

For baskets containing only rubble and fitted with a flexible seal the calculations indicate that 8% of the passivation flow would bypass the rubble through slots in the seal. Without the seal, bypass flow is calculated to increase to 46% of the total MCO gas flow. With a seal installed, placing fuel elements upright within the scrap basket increases the amount of bypass

flow from 8% for the rubble only case to 44% for 10 intact fuel elements (Figure 4-1). Figure 4-2 shows similar results for 10 partial (outer cylinder) elements. Here the bypass flow is seen to increase from 8% to 51%. Without the seal, bypass flow shown on Figure 4-1 is seen to increase from 46% to 61% with the addition of 10 intact fuel elements in the scrap basket. For partial fuel elements the same scrap basket configuration results in an increase in bypass flow from 46% to 66%, as shown on Figure 4-2.

Note that while the flow area for a fuel element outer cylinder is nearly twice that of an intact fuel element the increase in bypass flow for an equivalent number of elements in a scrap basket is much less (bypass flow increase from 44% for 10 intact fuel elements to 51% for 10 partial elements). This occurs because the perforations in the base plate of the scrap basket becomes the controlling resistance for flow through the fuel elements. Placing fuel elements in a scrap basket which does not have a seal between the basket side wall and the inside of the MCO will not increase the bypass flow as greatly as the case where the basket has a seal. This results from lower flow through the rubble bed producing pressure loss which is only slightly higher than that of the added fuel elements.

4.2 MCO SUB-CHANNEL FLOW DISTRIBUTION

Knowledge of the flow distribution within the MCO is necessary as a basis for design and operational decisions for the hot vacuum conditioning and passivation process. Flow distributions can determine the degree of conditioning uniformity, the time required for passivation, and the ability or accuracy by which the passivation process can be monitored. Initial flow distributions as presented in Section 4.1 were calculated using a one-dimensional flow network model which assumed that any radial pressure distribution within the MCO does not significantly affect the overall flow distribution. The COBRA-TF hydraulic model of the MCO is fully 3-dimensional and only makes the assumption that any circumferential flow will be negligible because of symmetry. Therefore, only a 30° sector about the central axis of the MCO need be modeled (see Figure 3-10). Each fuel storage basket is explicitly modeled, including each fuel rod, the internal and external flow passages, the base plate, half-height skirt and bypass area between the basket and MCO wall. The scrap baskets are modeled as a porous media with a full-height skirt and mechanical seal between the skirt and MCO wall. Both the axial and radial flow distribution is calculated for both geometries.

A comparison of the results from the two calculational methods is presented in the following table which compares the iso-thermal mass flow distribution through the scrap and fuel storage baskets. The comparison is given in percent of total flow through the MCO for an input flow rate of 10 SCFM of argon gas at an inlet temperature of 428 °F (220 °C).

Table 4-3. Network and COBRA-TF Mass Flow Comparison.

Code	Scrap Basket			Fuel Basket				
	Rubble (%)	Bypass (%)	Center Tube (%)	Centers (%)	Annuli (%)	Exteriors (%)	Bypass (%)	Center Tube (%)
Network Model	81	14	6	9	39	31	15	6
COBRA-TF	87	12	0.6	12	48	26	13	0.6

The COBRA-TF results listed in the table represent a summation of mass flow through all like channels (eg. all channels within the rubble). The very good comparison between the two models indicate that there is no gross radial flow distribution within the MCO. The relatively small differences in the two results are attributed to slight differences in how the two codes calculate the component pressure losses as well as the affect of some secondary radial flow redistribution which is described below.

The velocity distribution within the MCO predicted by the COBRA-TF model for the above case is presented in Figures 4-3 through 4-6. Figure 4-3 presents vertical velocities as a function of axial distance through the rubble bed and fuel center channels (See Figure 3-10 for an explanation of the channel numbers and Figure 3-9 for the axial node numbers). Velocities through the center channels of the fuel elements in the central region of the MCO appear to be very uniform and approximately 4 times higher than those in

comparable channels within the rubble. This is simply a result of the larger flow area represented by the porous media of the rubble. The small dip in velocity as the flow exits the top of the fuel elements in the bottom-most fuel storage basket represents some limited flow redistribution between the internal fuel channels and those channels exterior to the fuel in the region near the top of this basket. This represents only a 0.3% reduction in mass flow through the upper two baskets. Vertical flow velocity in the outlet plenum above the upper scrap basket will vary greatly depending upon the proximity of the flow channel to the exit (channel 13) in the MCO shield plug.

Similar results are shown on Figure 4-4 for those vertical flow channels which pass through the rubble and fuel outer annuli. Flow velocity in the rubble is seen to be the same as that shown on the previous figure, indicating uniform flow within the rubble. Flow velocity in the fuel outer annuli is seen to be approximately 3/4 of that through the central fuel channels. However, mass flow through these channels is roughly 4 times that of the center channels because of the five and a half times greater flow area.

The vertical flow velocities for channels exterior to the fuel and within the outer ring of fuel elements are shown on Figure 4-5. Flow velocities in this region are comparable to those in the rubble. The drop in velocity after the flow exits the base plate of each of the fuel storage baskets is the result of lateral flow redistribution to the larger flow channels associated with the outer ring of fuel elements near the MCO wall. Likewise, flow redistribution inward causes the flow increase at the entrance to the upper scrap basket. This lateral flow redistribution within the fuel storage baskets is shown in the outer channels on Figure 4-6. Velocity through the base plate of the storage baskets in these outer channels is seen to be relatively low but increases as flow from the inner channels as well as flow from the MCO bypass (Channels 28 and 29) enters this region. Toward the top of the basket the velocity in these channels then tends to drop as flow moves inward, or out toward the MCO wall.

The COBRA-TF results show that while the overall flow distribution through the MCO is relatively constant from basket-to-basket there is some mixing of the flow external to the fuel elements within each of the fuel storage baskets. This mixing process should be beneficial for both heat transfer and oxygen redistribution. However, because of the low purge gas flowrate the flow distribution within the MCO is very sensitive to small changes in operating pressure and temperature (gas density). Therefore, these iso-thermal results are expected to change appreciably as soon as a significant amount of heat is generated within the MCO. See Section 4.4.1 for a discussion of the process simulation results.

4.3 PASSIVATION REACTION LENGTH

4.3.1 Reaction Length for Complete Consumption of Oxygen

The length of fuel that can be passivated by a given oxygen flow is a function of the temperature of the fuel and the amount of fuel reaction area. Fuel that has a large surface area of uranium exposed to oxygen will consume a larger amount of oxygen than fuel which has little surface area of uranium exposed. The reaction length (length required to consume all of the oxygen in the inlet flow) as a function of temperature for oxygen volume fractions of 0.1%, 0.5%, 1%, 1.5%, 2% and 2.5% and a total gas flow of 10 cfm are shown in Figure 4-7 for a reaction surface area equivalent to the geometric surface area of 100% degraded Mark IV fuel. The reaction rate relationship is based on the modified Ritchie relationship discussed in Section 3.4.1.2.5. The vertical line in Figure 4-7 is drawn through 200 °C (473.16 °K). It can be seen from the plot that, at this temperature, some of the oxygen is left by the time the flow reaches the exit of the top fuel basket (about 10.9 feet of fuel). Higher oxygen concentrations could have greater fractions available by the time the flow reaches the top of the fuel. The oxygen would be consumed before exiting the fuel region if the fuel is at higher temperatures. There would still be some oxygen left in the fuel at lower temperatures.

The oxygen would be consumed at a faster rate over shorter lengths if the fuel reaction surface area is greater than the geometric surface area of completely degraded fuel. This effect is shown in Figures 4-8 and 4-9. Figure 4-8 presents the reaction length versus temperature for variable oxygen concentrations for a reaction area equal to 800,000 cm². Figure 4-9 presents the reaction length versus temperature for variable oxygen concentrations for a reaction surface area equal to 10 times (X) the geometrical surface area of completely degraded fuel. The reaction length for 0.1% oxygen for the 800,000 cm² case is approximately 8 feet (12 feet for 1.0% oxygen). The reaction length for the more conservative 10X case is less. All of the oxygen in a 0.1% mixture at a total flow of 10 cfm would be completely consumed in the first 4 feet of fuel at a temperature of 200 °C for a 10X fuel condition (16 feet for 1.0% oxygen). Such a condition may exist in the rubble baskets that are to be placed at the top and bottom levels of the MCO. It would be better if such damaged fuel could all be placed at the top of the MCO so oxygen would cover all of the less damaged fuel and passivate it before being completely consumed by the highly damaged, high surface area fuel.

The passivation process must be carried out at lower temperatures for a longer period of time if the reaction surface area is large to assure that all surfaces receive oxygen and are passivated. The oxygen in a 2%, 10 scfm flow will be totally consumed at the exit of an MCO containing fuel with a reaction area equal to 10X, the geometrical surface area of the fuel if fuel temperature is reduced to 190 °C.

The effect of fuel reaction surface area on oxygen reaction length is shown in Figure 4-10 for a total gas flow of 10 cfm and a fuel temperature of 200 °C. Clearly, as fuel damage increases the length of fuel required to consume all of the oxygen rapidly diminishes. The short reaction length fuel will consume all of the oxygen for a long period of time until all of the uranium is reacted. This means that fuel higher in the bundle will receive no

passivation at all during the time period that is allowed for hot passivation. It has already been shown in Section 3.4.1.2.1 of this report that it takes 1569 hours to react uranium to a depth of 2mm at 200 °C. The outer fuel element is over 9mm thick.

4.3.2 Heat Release Due to Oxidation Reaction

The reaction lengths presented in the previous section are based on constant fuel temperatures. No effort is made to evaluate how the fuel can be maintained at these temperatures. Maintaining the fuel at a constant temperature may be difficult if the heat released by the reaction becomes significant compared to the decay heat or the ability of the system to dissipate the heat. The heat release due to the oxidation reaction as a function of fuel temperature and fuel surface area is shown in Figure 4-11. Fuel having a reaction surface area equal to the geometric surface area of clad fuel, 1X, and having a temperature of 200 °C, will generate over 220 watts per lineal foot of fuel in a Mark IV fuel basket given an unlimited supply of oxygen.

The heat of reaction as a function of total gas flow and the volume fraction of oxygen is given in Figure 4-12 for a fuel temperature of 200 °C. The horizontal solid lines in the figure represent the average and maximum decay heats specified for the MCOs. The solid vertical line is drawn through a total gas flow of 10 cfm, the anticipated flow specification for hot conditioning. It can be seen from this figure that for a flow of 10 cfm, an oxygen volume fraction of 0.5% will generate more heat due to the reaction than the average MCO decay heat rate and nearly as much as the maximum MCO decay heat rate. An oxygen concentration of 2% at this flow and fuel temperature will generate over three times the maximum decay heat in reaction heat. This is of concern because, at these flows and temperatures, the fuel will become self heating since the system will not be able to reject heat faster than it is being generated. This will result in a temperature excursion in the fuel that will produce higher reaction rates and result in shorter reaction lengths.

The heating rate of the fuel for 2% oxygen and various surface area multipliers, assuming that all of the heat is stored in the fuel, is given in Figure 4-13a. The fuel is likely to heat several hundred degrees during the passivation period if heat rejection from the system is poor. Considerable thought will need to be given to the operating temperature of the fuel, the amount of oxygen to be supplied, and the amount of fuel reaction surface area that exists in the MCO. Figure 4-13b shows the heating rate of fuel assuming all of the reaction energy is deposited in the fuel for various oxygen concentrations with a 1X surface area multiplier.

4.3.3 Time to Achieve Reaction Depth

The objective of the passivation step during hot conditioning is to remove as much of the freshly exposed uranium that is created by the dehydriding step as is possible. Some understanding of the time required to achieve this can be obtained by estimating the time required to react a certain depth of uranium on the fuel surface. A plot of this reaction time

versus depth on the surface of the fuel rod is shown in Figure 4-14. The fuel can be oxidized to a depth of only 3 μm in approximately 16 hours at a fuel temperature of 200 °C. Freshly exposed uranium surfaces that are thicker than this will not be completely passivated. The effect of increased reaction surface area (i.e., 10X), as shown by Figure 4-15, is to increase the depth that will be reacted in a given amount of time assuming sufficient oxygen is available to sustain the reaction.

Careful consideration will need to be given to the temperatures the fuel is to be passivated at to insure that:

1. Sufficient and a uniform distribution of oxygen reaches all exposed fuel surfaces such that highly reactive uranium metal is not left unpassivated in the MCO. This could occur if highly damaged fuel in the lower elevations of the MCO consume all of the oxygen before it reaches the upper elevations of the MCO. This process may not be controllable for highly damaged fuel or scrap since any reaction that starts will continue as long as oxygen is supplied or until all the oxygen is consumed.
2. The heat of reaction will be the dominant heat source at higher fuel temperatures. This may cause the fuel to melt during passivation, shortening the reaction length and resulting in the fuel higher in the bundle not being passivated. The reaction heat may also make the process hard to control if the heat cannot be adequately dissipated.

4.4 HCS THERMAL-HYDRAULIC PERFORMANCE

4.4.1 Process Simulation With Integrated COBRA-TF Model

Two thermal transients associated with the passivation process were run using the integrated COBRA-TF model of the MCO. The transient calculations simulated initiation of the passivation process with the objective of verifying the oxygen consumption predictions of the one-dimensional scoping models described in Section 4.3.1 and to determine the effect any flow redistribution will have on oxygen consumption and internal temperatures.

The COBRA-TF calculations simulated the effect of two different initial temperatures on the passivation process. Both calculations assume the MCO is installed in the hot vacuum conditioning station and that the hot conditioning process step has been completed with MCO temperatures reduced and stabilized at the initial conditions for the passivation step (No radial or axial temperature gradients within the MCO). The temperature of the inert purge gas and the temperature of the gas in the jacket surrounding the MCO are assumed to be the same and that both remained constant throughout the passivation transient. The flow rate of the argon purge gas into the MCO was set at 10 scfm. The passivation step is initiated by the introduction of oxygen into the purge gas at a 2% by volume concentration.

Fuel elements and scrap within the MCO have been assumed to have a decay heat equivalent of 3.44 watts per element (929 w/MCO with 5 tiers of 54 elements each). Porosity of the rubble within the scrap baskets is chosen to be 0.46 with a mean particle diameter of 3/4 inch. Thermal radiation within the rubble filled scrap baskets is based on an emissivity of 0.43. Reactive surface area of the rubble in each basket is set to 800,000 cm², independent of the assumed porosity. In addition it is assumed that the top 6 inches of each fuel element is corroded with a reactive surface area equal to 10 times the geometric area.

The first transient calculation assumes a passivation process temperature of 100 °C (212 °F) with 2% oxygen in the inert purge gas flow. The one-dimensional calculations (Figure 4-8) indicated that the reaction length required to consume all of the oxygen for fuel at this temperature is much greater than the overall length of the MCO. However, decay heat was expected to raise the fuel temperatures sufficiently such that some of the oxygen would be reacted within the MCO. The COBRA-TF calculations are to indicate how much of the oxygen would be reacted and where within the MCO the reactions occur.

Results for this case (100 °C) are interesting because the oxidation reaction is predicted to start in the upper scrap basket (Figure 4-16). The oxidation reaction starts first near the top surface of the upper scrap basket because decay heat is transported from the fuel in the lower portion of the MCO to the upper scrap basket by the purge gas. This results in the highest fuel temperatures at the top of the MCO and hence the highest chemical reaction rates. This thermal transient is predicted to progress fairly slowly at first because of the low temperatures associated with the initial conditions and the large heat capacity of the fuel.

Purge gas temperatures as a function of axial position within the MCO are shown on Figures 4-16, 4-17, and 4-18 after 30 hours of processing. The relationship between axial node numbers and position of the various fuel and scrap baskets within the MCO is shown in the COBRA-TF model diagram in Figure 3-9. Note that the fuel temperatures are very close to the gas temperatures shown on Figure 4-16. This occurs because of the relatively low gas flow rate and the large surface area associated with the fuel (see the corresponding fuel temperatures for the scrap baskets and central fuel assemblies on Figures 4-19 and 4-20). MCO structural temperatures are shown on Figure 4-21. Note that the end points of the temperature curves for the support rods and basket base plate indicate temperatures less than 200 °F. This is only an artifact of the plotting program. The purge gas temperature rises approximately 90 °F through the lower scrap basket to 300 °F at the top surface of the rubble. The reaction length model (Figure 4-8) indicates that this temperature is too low to induce any significant oxidation reaction. Heatup of the purge gas across the next three fuel baskets is seen to be approximately 50 °F. The increasing spread in channel temperatures shown on the figure in the region of the fuel baskets indicates that an approximate 40 °F radial gradient is established between the inner fuel elements and those near the MCO wall. Gas temperature entering the upper scrap basket is approximately 350 °F. At this temperature a significant oxidation reaction would be expected to occur (Figure 4-8). The COBRA-TF calculations indicate that this indeed is the case by the large temperature rise through the upper scrap basket. At the peak rubble temperature shown on the Figure 4-19 (460 °F) the reaction length required to use up all the oxygen is less than 3 feet. The integrated effect of the temperature rise through the scrap basket should therefore result in essentially all of the oxygen entering the scrap basket being consumed. The COBRA-TF predictions for oxygen concentration in the rubble and intact fuel elements as a function of axial position is shown on Figure 4-22. This figure shows that very little oxygen is consumed in the lower scrap basket and in next three fuel baskets. However, as the purge gas traverses the upper scrap basket the oxygen concentration is calculated to decrease from 1.7% at the bottom of the basket to 0.2% at the top. The increase in oxygen concentration to 0.9% between the top of the upper rubble basket and the MCO outlet is due to mixing with the purge gas which bypassed around the outside of the upper scrap basket as shown on Figure 4-23, where channels 28 and 29 represent the basket bypass. Note that a significant oxidation reaction occurring in the upper basket would be difficult to verify using an outlet oxygen monitor because of the effect of the bypass flow on outlet oxygen concentration.

As presented in Figures 4-17 and 4-18 the calculated purge gas temperatures along the exterior surfaces of the intact fuel elements shows a saw-tooth shaped temperature variation. This variation results from mixing with cooler gas flowing next to the MCO wall (channels 28 and 29 on Figure 4-18). Flow channels near the MCO wall have the largest temperature variation while those near the center of the MCO show almost none.

As indicated on the figures, these calculations present the state of the MCO after approximately 30 hours of operation. Temperatures within the upper scrap basket are predicted to continue to increase with time and the position of the peak temperature to progress downward in the basket until all of the available oxygen is consumed. It appears that this situation will always occur for large reaction surface areas because the heat removal capability of

the MCO is limiting compared with the heat generation rate of the oxidation reaction. This is illustrated by the temperatures predicted for this case four hours later (after 34 hours of operation) as shown on Figure 4-24. Peak temperature in the upper scrap basket has increased 220 °F to 700 °F and its position within the scrap basket has moved downward nearly 8 inches. Oxygen concentration within the MCO is shown on Figure 4-25 indicating that essentially all of the oxygen entering the upper scrap basket is being consumed. The outlet oxygen concentration has decreased to 0.3% by this time due to spreading of the "hot spot" to include all of the basket. Note that as the hot spot moves downward in the rubble due to heat conduction it will probably tend to concentrate resulting in higher temperatures than those shown on Figure 4-24. Therefore, it is entirely possible that for these large reaction areas temperatures could exceed the melting point of the fuel.

The second thermal transient assumed a passivation inlet process temperature of 230°C (446 °F). At this process temperature the one-dimensional reaction length calculations (Figure 4-8) indicate that a significant oxidation reaction should occur. In this case the chemical reaction should be concentrated in the lower scrap basket and, based on the results of the first case, the reaction rate should increase the temperature of the rubble until all of the oxygen passing through the rubble is consumed.

The COBRA-TF predictions after 40 hours of operation are shown on Figures 4-26 through 4-33. Figure 4-26 shows a plot of the purge gas temperatures as a function of axial node location through the length of the MCO (see Figure 3-9 for a nodal diagram of the MCO). Again, because of the low purge gas flow rate, the gas temperatures and fuel temperatures are nearly equal. This can be seen by comparing Figure 4-26 with Figures 4-29 and 4-30 which present the rubble and fuel rod temperatures, respectively. Note that the peak temperature of nearly 1150 °F occurs near the base of the bottom rubble basket and that the temperature then decreases over the remaining length of the MCO with an outlet temperature of 580 °F. Gas temperatures around the outside of the intact fuel elements are shown on Figure 4-27 and 4-28. The variation in temperature around these elements is the result of mixing with the cooler purge gas which flows up along the MCO wall (channels 28 and 29 in Figure 4-28). Structural temperatures within the MCO are shown on Figure 4-31. In this figure note that the MCO wall temperature peaks at about 550 °F while the adjacent rubble temperatures are approximately 1150 °F. Note also that the connection of the support rod and basket base plate temperatures to values less than 400 °F at the end points of the curves is an artifact of the plotting program. The reason for the decreasing temperature over the length of the MCO is that all of the oxygen passing through the rubble in the lower scrap basket is used up within the first few inches as seen in Figure 4-32. Oxygen bypassing the lower scrap basket is mixed with the oxygen depleted purge gas exiting the basket and is progressively reacted with damaged end surfaces of the fuel rods in the next three baskets (see Figure 4-33). There is essentially no oxygen reaching the upper scrap basket or MCO outlet.

Other than the depletion of oxygen, this case will be difficult to detect with the currently planned instrumentation because the outlet temperature rises very slowly. The large heat capacity of the fuel and MCO structure act as a very good heat sink and therefore limits the effectiveness of the outlet temperature instrumentation. The approximate 130 °F temperature

rise in the outlet temperature may be sufficient to indicate a problem after 40 hours of operation. However, after 20 hours of operation (Figure 4-34) peak temperatures are nearly the same as those described above but the outlet temperature change is now only 40 °F. This small amount of temperature rise would not normally indicate a problem even though one may actually exist.

4.4.2 Process Simulation With Simplified COBRA-TF Model

Two thermal transients associated with the passivation process were run using the simplified COBRA-TF ring model of the MCO. The first transient simulates the heatup and cooldown portions of the entire HCS process (Figure 1-2) for an average powered MCO with helium as the purge gas. Chemical reactions are not modeled as part of this simulation. The MCO fuel and structure temperature versus time are shown in Figure 4-35. The transient was assumed to commence from an initial temperature of 302 °F (150 °C).

For the first 32 hours, the Dewar (jacket) wall leads the fuel and structure temperatures due to the increasing temperatures of the surrounding Dewar flow, which is assumed to ramp up from 302 °F (150 °C) to 572 °F (300 °C) over 12 hours. By 60 hours, equilibrium temperatures are nearly obtained, with the maximum temperatures now in the center support tube and inner fuel. After 72 hours, when the surrounding Dewar gas temperature is assumed to have ramped down for 12 hours at 12.5 °C/h, the peak fuel temperatures remain significantly higher (+150°F) than the Dewar wall. This is due to large heat capacity associated with the uranium fuel and the poor heat transfer rates within the MCO. After 84 hours, the peak fuel temperatures are approximately 80 °F greater than the Dewar wall.

The second transient simulates the first 54 hours of the HCS process for an average powered MCO with argon as the purge gas. Again, chemical reactions are not modeled. The MCO fuel and structure temperatures versus time are shown in Figure 4-36. The transient is assumed to commence from a uniform initial temperature of 50 °F (10 °C).

Because of the poor thermal conductivity of argon relative to helium, the rate of fuel heatup is much slower than the helium case as presented in Figure 4-35. Conversely, the rate of fuel cooldown will be much longer than the helium case. In addition, the temperature difference between the inner fuel and the dewar wall is greater with argon. In general, the effective heat transfer rate associated with argon is significantly less than helium, resulting in much larger temperature differences across the baskets and an increased time to complete the process.

The results for these two cases are interesting because of the non-uniform temperature distribution across the fuel basket and the peak fuel temperature associated with the inner fuel assemblies. This is of concern because, with chemical reactions, at these flows and temperatures, the inner fuel assemblies will become self heating, since the system has a significant time lag before it will be able to reject heat faster than it is being generated. This will result in a temperature excursion in the fuel. Cooldown periods longer than 12 hours that result in a more uniform temperature distribution must be investigated, as well as, a potential ramp for oxygen concentration during the passivation portion of the HCS process.

4.4.3 Scrap Basket Thermal Performance and Process Simulation With Detailed Tier Model

A series of steady-state and transient analyses were performed to determine the thermal-hydraulic performance characteristics of a scrap basket. The FIDAP thermal-hydraulic model of the scrap basket was used to perform the analyses. The subject thermal-hydraulic model is a fully three-dimensional 30° sector representation of a full height scrap basket with the assumption that any circumferential flow will be negligible because of symmetry. The scrap basket was assumed to occupy the lowest tier within the MCO and was completely filled to the maximum depth of 26.1 inches with rubble. The scrap basket was modeled as a homogenous porous media with a full-height skirt and mechanical seal between the skirt and MCO wall. The energy gains to the scrap basket were modeled as a constant nuclear decay heat source and a temperature and oxygen concentration dependent chemical reaction rate heat source based on the modified Ritchie relationship discussed in Section 3.4.1.2.5 for a value of n equal to 0.77. A total reactive surface area equivalent to 800,000 cm² (80 m²) per scrap basket is assumed for all the analyses. The nuclear decay heat of the fuel rubble is assumed to be identical to intact fuel and is varied from minimum to maximum values multiplied by the value (1-POROSITY), where porosity is assumed to range from 0.259 to 0.476. (These values represent the minimum and maximum porosity values for uniform sized spherical particles stacked in cubical pattern.) The purge or carrier gas is assumed to be either helium or argon with oxygen concentrations ranging from 0.5% to 10% by volume.

The flowrate through the porous scrap material is reduced to account for 13% bypass flow around the scrap basket and is based on a total flowrate of 10 scfm. The 13% bypass flow assumes flow restrictors within the radial gap and the center tube was assumed to be a high resistance flow path. The actual analyses assumes that the small radial gap between the outer diameter of the basket skirt and inner diameter of the MCO and the volume within the center support pipe is stagnate.

The HCS Dewar or MCO-to-jacket gap flow was based on a total flowrate of 250 scfm, with an inlet temperature of 423.16 °K. For the transient simulation of the HCS dehydrating process, as shown in Figure 1-2, the Dewar flowrate was assumed to remain at 250 scfm. The inlet temperature for both the Dewar and MCO purge flow was assumed to ramp up from 423.16 °K to 573.16 °K (300 °C, 572 °F) over 12 hours, remain at 573.16 °K for 48 hours, then ramp down to 423.16 °K over 12 hours. The initial temperature for the entire model was assumed to 423.16 °K. The passivation step was assumed to begin after the cooldown at 72 hours holding at an inlet temperature of 423.16 °K for an additional 12 hours while 2% oxygen was added to the purge gas.

Table 4-4 presents a summary of the steady-state peak temperatures that have been obtained for minimum decay heat and minimum porosity (maximum effective thermal conductivity) scrap basket with helium as the purge gas. Figures 4-37 through 4-44 present the corresponding temperature contours from Table 4-4. (Table 4-4 also presents a footnote summary of the peak temperature results for two maximum decay and maximum porosity (minimum effective thermal conductivity) scrap basket cases with helium as the purge gas.) Table 4-4 indicates that for oxygen concentrations greater than 2% by

volume the peak temperature increase dramatically. The peak temperature of the 2% oxygen case is 457.9 °K (364.5 °F) versus the 3% oxygen case with a peak temperature of 581.5 °K (587.0 °F). Between 2.0% and 3.0% oxygen by volume a significant temperature increase occurs. For the maximum decay heat, maximum porosity cases, this temperature increase occurs between 0.5% and 1.0% oxygen. This rapid increase in peak temperatures is an indication that the energy removal capability of the scrap basket is being challenged and that steeper temperature gradients are required to promote energy removal. The increased temperature associated with these gradients leads to increased local reaction rate and oxygen consumption. The reaction front eventually begins to progress downward through the scrap towards the maximum oxygen concentration as shown in Figures 4-41 through 4-44. The maximum decay heat and maximum porosity helium case results indicate a peak temperature of 469.7 °K (385.8 °F) and 581.7 °K (587.4 °F) for 0.5% and 1.0% oxygen by volume. This is significantly higher than the corresponding minimum case and is indicative of the higher temperature associated with maximum decay heat and the degraded effective thermal conductivity due to the increased porosity. (See Figure 3-23 for a comparison of the effective thermal conductivity for helium for porosities of 0.259 and 0.476.) As with the minimum decay heat and porosity cases the reaction front eventually begins to progress downward through the scrap basket towards the maximum oxygen concentration (Figures 4-53 through 4-56), due the higher temperatures associated with maximum decay heat and a degraded thermal conductivity, the progression occurs at lower oxygen concentrations.

Figures 4-45 through 4-52 present the corresponding oxygen concentration (species 1) contours from Table 4-4 for a minimum decay heat scrap basket with a minimum porosity of 0.259 with helium as the purge gas and for oxygen concentrations ranging from 0.5 to 10% by volume. This combination of conditions results in the maximum effective thermal conductivity possible for a scrap basket with helium as the purge gas and the minimum possible temperature rise due to decay heat. The thermal response of the scrap basket with helium as the purge gas cannot get any better than this.

Figures 4-53 through 4-56 present the corresponding temperature and oxygen concentration contours from Table 4-4 for a maximum decay heat scrap basket with a maximum porosity of 0.476 with helium as the purge gas during the passivation phase for oxygen concentrations ranging from 0.5 to 1.0% by volume. This combination of conditions results in the minimum effective thermal conductivity possible for a scrap basket of packed spheres with helium as the purge gas and the maximum possible temperature rise due to decay heat for the range of porosities studied. These figures confirm the same trend as the COBRA-TF argon simulations, as discussed in Section 4.4.1, with regard to the downward progression of the reaction front towards increasing oxygen concentrations and higher temperatures for helium rather than argon. The same downward progression effect occurs for the range of helium conditions. Since the reaction rate is dependent on both the local temperature and oxygen concentration, increasing either the local temperature or oxygen concentration results in the same downward progression of the reaction front towards higher oxygen concentrations. The temperature dependency is much stronger, because of the exponential term in the reaction rate relationship. The oxygen dependency is weaker and is based on the local oxygen concentration raised to a power of 0.77. These findings are of course based on current knowledge for

the governing heat production and energy removal capabilities of the MCO within the HCS.

Figure 4-57 presents the temperature versus time for locations within the scrap basket that were obtained for the 72 hour HCS dehydrating process simulation for an argon purge flow, nominal decay heat and a porosity of 0.476. Figures 4-58 and 4-59, respectively, present the temperatures for the same series of nodes, but for the first 36 hours during the heatup portion and the last 36 hours during the cooldown portion. This analysis obtained an estimate of both the maximum fuel temperatures and response time to heatup and cooldown prior to the entering the passivation interval. Nodes 380, 378, 410, 408, 429, 427, 437, 422, and 384 correspond to evenly spaced location across the upper face of the scrap basket progressing the innermost scrap node (380) to the outermost scrap node (384). Nodes 5699 and 1012 correspond to the inlet temperature for the Dewar or Jacket flow and MCO purge flow, respectively, and reflect the programmed temperature ramp. Node 42 corresponds to the outlet temperature of the Dewar flow. No chemical reaction are assumed during the 72 hour transient HCS process simulation. Note that during the heatup phase of the HCS process simulation the outer perimeter of the scrap basket (Node 384) is at a higher temperature than the interior (Node 380). The reverse is true after approximately 30 hours. The interior portions of the scrap basket are at higher temperature than the perimeter.

Approximately 42 hours are necessary to obtain equilibrium conditions within the scrap basket with argon as the purge gas. Note that the effective thermal resistance of the scrap basket is less than a fuel basket with fuel elements surrounded by argon. The scrap basket has a lower time constant. Intact fuel will take longer to heatup and cooldown. The use of argon may not provide enough time to complete the dehydrating phase within the scrap basket, as well as the fuel basket, prior to reaching the end of the 48 hour (60 hours total) dehydrating phase. This must be investigated for the fuel basket prior to committing to the proposed HCS process.

Figures 4-60 through 4-69 present the temperature contours expected at 3, 6, 9, 12, 36, 60, 63, 66, 69, and 72 hours, respectively, during the HCS simulation. Figure 4-69 indicates that at 72 hours after 12 hours of cooldown a temperature gradient of approximately 160 °K (288 °F) exists within the scrap basket. This gradient is large enough to result in a chemically reactive hot spot given the presence of oxygen if the passivation phase was commenced at this time. Process cooldown times longer than 12 hours are necessary to decrease the thermal gradients within the scrap basket. Process times greater than 72 hours with argon have not yet been investigated. However, process times greater than 72 hours with helium have been investigated and are discussed with the following paragraphs.

Figure 4-70 presents the scrap temperatures versus time for various locations within the scrap basket. These temperatures were obtained for a 84 hour HCS process simulation of a scrap basket with helium as the purge gas, nominal decay heat, and a porosity of 0.476. The proposed 72 hour HCS process time, plus an additional 12 hour hold at an inlet temperature of 423.16 °K (302 °F), was simulated to determine the decrease in the temperature gradients within the scrap basket and MCO due to a longer process time. Figures 4-71, 4-72, and 4-73, respectively, present the temperatures for the same series of

nodes as above, but for the first 36 hours, the last 48 hours (36 to 84 hours), and, finally, the last 24 hours (60-84 hours) during the 12 hour cooldown and 12 hour hold. No chemical reactions are assumed during the 84 hour HCS process simulation. Note that during the heatup phase of the HCS the outer perimeter of the scrap basket (Node 384) is at a higher temperature than the interior (Node 380). The reverse is true after approximately 22 hours. The interior portions of the scrap basket are at higher temperature than the perimeter. Approximately 28 hours are required to reach equilibrium conditions within the scrap basket with Helium. This is significantly less than the 42 hours required given argon as the purge gas. Note that the effective thermal resistance of the scrap basket is less than a fuel basket with fuel elements surrounded by helium. The scrap basket has a lower time constant. Intact fuel will take longer to heatup and cooldown. The use of helium as the purge gas appears to provide enough time to complete the dehydriding phase within the scrap basket. However, this remains to be confirmed for the fuel basket prior to committing to the proposed 48 hour HCS dehydriding phase.

Figures 4-74 through 4-93 present the temperature contours expected at 3, 6, 9, 12, 18, 24, 30, 36, 42, 48, 54, 60, 63, 66, 69, 72, 75, 78, 81 and 84 hours, respectively, during the 72 hour HCS process and 12 hour hold simulation. Figures 4-89 and 4-93, respectively, indicate that after 12 hours of cooldown (72 hours process time) a temperature gradient of approximately 84 °K (150 °F) exists, decreasing to approximately 21 °K (38 °F) at the end of the 12 hour hold (84 hours process time). The thermal gradients for helium are much smaller than the corresponding argon cases. However, if the passivation phase began at 72 hours, the 150 °F temperature gradient from Figure 4-89 is still large enough to result in a chemically reactive hot spot, but not after an additional 12 hour hold. The proposed 12 hour hold may not be long enough for the fuel basket containing fuel assemblies. A longer hold period might be required. This must be investigated prior to modifying or extending the HCS process cooldown time.

In summary, the results of the three-dimensional scrap basket analyses indicate that the proposed HCS cooldown time of 12 hours for the HCS simulation with either argon or helium as purge gases does not appear to be sufficiently long for the temperature gradients to decrease enough within the interior of the scrap basket to avoid creating chemically active hot spots during the passivation phase. In particular, for argon from Figure 4-69, a temperature difference of approximately 160 °K (288 °F) exists at the end of the 12 hour cooldown. A significantly longer time will be required to minimize the temperature gradients with argon as the purge gas. For helium temperature gradients of approximately 84 °K (150 °F) exist at 72 hours; decreasing to approximately 21 °K (38 °F) at the end of the 12 hour hold. The assumed 12 hour hold (i.e., 72 + 12 hours) at an inlet temperature of 423.16 °F (302 °F) appears to be adequate given helium as the purge gas for minimizing temperature gradients prior to commencing the passivation phase. Because the effective thermal resistance of the scrap basket is less than fuel baskets, the proposed 12 hour hold may not be adequate for fuel baskets. A longer hold period might be required. This must be investigated prior to modifying or extending the HCS process cooldown time.

These analyses confirm the same trends as the COBRA-TF helium and argon results presented in Figures 4-35 and 4-36. The proposed 12 hour heatup and

cooldown does not appear to be sufficient, given either argon or helium, to minimize the temperature gradients within the fuel baskets prior to commencing the passivation phase.

Estimates of the heat transfer coefficient across surfaces adjacent to flow fields were derived from the above transient simulations. These values are presented in Tables 4-5 and 4-6. The subject three-dimensional scrap basket model does not require an explicit heat transfer coefficient for solid surfaces adjacent to a flow field. A convective heat transfer coefficient is required for those surfaces (i.e., external) where the adjacent flow field is not explicitly calculated, such as the outermost exterior wall exposed to ambient conditions. The effective heat transfer coefficient, incorporating both diffusive and convective heat transfer, was derived by performing an energy balance across the surface of interest as discussed in the following paragraphs.

Pointwise total heat transfer coefficients, h_c ($J/m^2 \cdot s \cdot ^\circ K$), are derived using the following equation:

$$h_c = q/A(T - T_{REF}) \quad (4-1)$$

Where, T_{REF} ($^\circ K$) is the assumed reference temperature of $302^\circ F$ ($423.16^\circ K$), T ($^\circ K$) is the temperature associated with each of the Gaussian integration points on the user selected surface or boundary of interest, and q/A ($J/m^2 \cdot s$) is the pointwise heat flux due to conduction and convection across the given elemental surface or boundary of interest at a given time during the simulation.

For isotropic thermal conductivity, the heat flux can be expressed as follows;

$$\frac{q}{A} = -\left(k \frac{\partial T}{\partial x_j}\right) n_j + \rho C_p V_i T n_i \quad (4-2)$$

Where, k = Isotropic thermal conductivity ($J/m \cdot s \cdot ^\circ K$) of the conductive solid or fluid.

∂x_j = Radial distance (m) between the Gaussian integration points lying on the elemental sides adjacent to the user requested surface or boundary and the corresponding surface.

∂T = Radial temperature ($^\circ K$) difference between the Gaussian integration points lying on the elemental sides adjacent to user requested surface or boundary and the correspond surface.

n_i, n_j = Normal unit vectors (orthogonal to each other) corresponding to the Gaussian integration points on the user selected surface or boundary.

ρ = Density (kg/m^3) of the convective fluid.

C_p = Specific heat ($J/kg \cdot ^\circ K$) of the convective fluid.

V_i = Axial velocity (m/s) of the convective fluid at the Gaussian points lying on the elemental sides adjacent to user requested surface or boundary.

T = Temperature ($^{\circ}\text{K}$) of the convective fluid at the Gaussian points lying on the elemental sides adjacent to user requested surface or boundary.

The first term in Equation 4-2 is referred to as the diffusive heat flux. The second term is referred to as the convective heat flux.

Using Equation 4-2 first, the pointwise heat fluxes are calculated using values associated with the Gaussian integration points. Next using Equation 4-1, the pointwise total heat transfer coefficient is calculated by dividing the pointwise total heat flux by the difference between the temperature associated with each of the Gaussian integration points on the subject surface or boundary and a reference temperature. An average heat transfer coefficient h_c ($\text{J/m}^2\text{-s-}^{\circ}\text{K}$) across the surface is obtained by integrating over the elemental areas and dividing by the total area.

Average values of the total heat transfer coefficient (h_c) are presented in Tables 4-5 and 4-6 for the MCO outer diameter (MCO OD) and the scrap basket skirt inner diameter (SKIRT ID) for an argon and helium purge flow, respectively, with nominal decay heat and a porosity of 0.476. A 12 hour cooldown period was assumed for the argon case as presented by Table 4-5. A 12 hour cooldown followed by a 12 hour hold at 423.16°K (302°F) was assumed for the helium case as presented by Table 4-6. Note that positive values indicate heat flow into the component (MCO or SKIRT) across the surface of interest. Negative values indicate heat flow out of the component across the surface of interest.

Both Tables 4-5 and 4-6 indicate that heat transfer occurs from the Dewar flow into the MCO wall and from the SKIRT into the scrap. During the 48 hour dehydriding phase, the total heat transfer coefficients decrease to low values then change signs indicating that a reverse temperature gradient has been established across the MCO with the higher temperatures within the scrap basket near the inner diameter (i.e., the scrap basket has obtained a equilibrium condition). During the cooldown portions, the total heat transfer coefficients increase significantly, indicating a much larger temperature gradient has been established across the scrap basket and MCO as energy is removed from the peripheral regions. The total heat transfer coefficients for both the argon and helium analyses show the same transient trends. However, the total heat transfer coefficients for helium, as presented in Table 4-6, are greater than the corresponding values for argon, as presented in Table 4-5. This is due to the increased thermal conductivity of helium relative to argon.

Table 4-4. Peak Fuel Temperatures for a Scrap Basket With Minimum Decay Heat, Minimum Porosity (0.259), and Helium Purge Gas.

Volume (%O ₂)	Mass Fraction O ₂	Peak Temperature* °K (°F)
0.5	0.03862	433.2 (320.1)**
1.0	0.07471	437.3 (327.5)**
1.5	0.10852	443.5 (338.6)
2.0	0.14026	457.9 (364.5)
3.0	0.19822	581.5 (587.0)
4.0	0.24985	594.0 (609.5)
5.0	0.29613	605.4 (630.0)
10.0	0.47039	633.3 (680.3)

* T_{IN} = 423.16 °K.** Corresponding peak fuel temperatures for maximum decay heat and maximum porosity (0.476) with a helium purge gas are 469.7 °K (385.8 °F) for 0.5% O₂ and 581.7 °K (587.4 °F) for 1%.

Table 4-5. Derived Total Heat Transfer Coefficients from Scrap Basket HCS Process Simulation for Argon Purge, Nominal Decay Heat, and Porosity = 0.476.

Inlet Temperature °K (°F)	Process Time s (hr)	Average* Heat Transfer Coefficient,** h _c (J/m ² -s-°K)	
		MCO_OD***	SKIRT_ID***
460.66 (370.0)	10800 (3)	+4.33	-4.22
498.16 (437.0)	21600 (6)	+2.60	-2.87
535.66 (505.0)	32400 (9)	+1.92	-2.18
573.16 (572.0)	43200 (12)	+1.37	-1.70
573.16 (572.0)	86400 (24)	-0.09	+0.13
573.16 (572.0)	129600 (36)	-0.16	+0.27
573.16 (572.0)	172800 (48)	-0.16	+0.28
573.16 (572.0)	216000 (60)	-0.16	+0.28
535.66 (505.0)	226800 (63)	-1.50	+1.10
498.16 (437.0)	237600 (66)	-2.56	+1.86
460.66 (370.0)	248400 (69)	-4.72	+2.82
423.16 (302.0)	259200 (72)	-7.76	+5.23

*

Axially integrated over 26.1 inches (0.66294 m) and averaged over surface area of interest.

** To convert from J/m²-s-°K to Btu/ft²-hr-°F multiply column values by 0.17612.

*** Positive values indicate heat flow into the surface of interest. Negative values indicate heat flow out of the surface of interest.

+(MCO_OD)=Heat flow into MCO from DEWAR flow; +(SKIRT_ID)=Heat flow into SKIRT from SCRAP

-(MCO_OD)=Heat flow from MCO into DEWAR flow; -(SKIRT_ID)=Heat flow from SKIRT into SCRAP

**Table 4-6. Derived Total Heat Transfer Coefficients from Scrap Basket
HCS Process Simulation for Helium Purge, Nominal Decay Heat,
and Porosity = 0.476.**

Inlet Temperature °K (°F)	Process Time s (hr)	Average* Heat Transfer Coefficient hc(J/m ² -s-°K)**	
		MCO_OD***	SKIRT_ID***
460.66 (370.0)	10800 (3)	+7.44	-8.03
498.16 (437.0)	21600 (6)	+4.61	-5.00
535.66 (505.0)	32400 (9)	+3.33	-3.56
573.16 (572.0)	43200 (12)	+2.38	-2.62
573.16 (572.0)	64800 (18)	-0.12	+0.12
573.16 (572.0)	86400 (24)	-0.22	+0.35
573.16 (572.0)	108000 (30)	-0.28	+0.43
573.16 (572.0)	129600 (36)	-0.29	+0.45
573.16 (572.0)	151200 (42)	-0.29	+0.45
573.16 (572.0)	172800 (48)	-0.29	+0.45
573.16 (572.0)	194400 (54)	-0.29	+0.45
573.16 (572.0)	216000 (60)	-0.47	+0.56
535.66 (505.0)	226800 (63)	-2.23	+2.04
498.16 (437.0)	237600 (66)	-3.89	+3.42
460.66 (370.0)	248400 (69)	-6.68	+5.28
423.16 (302.0)	259200 (72)	-17.31	+8.55
423.16 (302.0)	270000 (75)	-22.58	+12.49
423.16 (302.0)	280800 (78)	-22.62	+12.38
423.16 (302.0)	291600 (81)	-22.37	+12.07
423.16 (302.0)	302400 (84)	-22.14	+11.77

* Axially integrated over 26.1 inches (0.66294 m) and averaged over surface area of interest.
 ** To convert from J/m²-s-°K to Btu/ft²-hr-°F multiply column values by 0.17612.
 *** Positive values indicate heat flow into the surface of interest. Negative values indicate heat flow out of the surface of interest.
 +(MCO_OD)=Heat flow into MCO from DEWAR flow; +(SKIRT_ID)=Heat flow into SKIRT from SCRAP
 -(MCO_OD)=Heat flow from MCO into DEWAR flow; -(SKIRT_ID)=Heat flow from SKIRT into SCRAP

Figure 4-1. Scrap Basket Bypass Flow for Intact Fuel Elements.

Figure 4-2. Scrap Basket Bypass Flow for Fuel Assembly Outer Elements.

Figure 4-3. Vertical Velocity in Rubble and Fuel Central Channels.

Figure 4-4. Vertical Velocity in Rubble and Fuel Annular Channels.

Figure 4-5. Vertical Velocity in Rubble and Fuel Exterior Central Channels.

Figure 4-6. Vertical Velocity in Rubble and Fuel Exterior Edge Channels.

Figure 4-7. Length for Complete Reaction Versus Temperature for an Argon Gas Flow of 10 CFM and Reaction Area Equal to That of Declad Fuel Using Modified Ritchie for Oxygen Concentrations from 0.1% to 2.5% by Volume.

Figure 4-8. Length for Complete Reaction Versus Temperature for an Argon Gas Flow of 10 CFM and Reaction Area Equal to 800,000 cm^2 Using Modified Ritchie for Oxygen Concentrations from 0.1% to 2.5% by Volume.

Figure 4-9. Length for Complete Reaction Versus Temperature for a Nitrogen Gas Flow of 10 CFM and Reaction Area Equal to 10X That of Declad Fuel Using Modified Ritchie for Oxygen Concentrations from 0.1% to 2.5% by Volume.

Figure 4-10. Length for Complete Reaction Versus Reaction Surface Area for a Gas Flow of 10 CFM and Fuel Temperature of 473 °K (200 °C) Based on Modified Ritchie.

Figure 4-11. Lineal Heat Generation Rate Due to Oxygen Oxidation Reaction Versus Fuel Temperature Based on Ritchie.

Figure 4-12. Total Heat Generation Rate for Complete Reaction of Available Oxygen Versus Pump Volumetric Flow Given an Exit Fuel Temperature of 473 °K (200 °C).

Figure 4-13a. Heating Rate Assuming All Reaction Energy is Deposited in the Fuel for a Constant 2% Oxygen Concentration.

Figure 4-13b. Heat Rate Assuming All Reaction Energy is Deposited in the Fuel for the Complete Consumption of Various Oxygen Concentrations.

Figure 4-14. Time to React Fuel to a Specified Depth as a Function of Temperature for a Reaction Area Equal to that of Declad Fuel Using Modified Ritchie Assuming a Constant 2% Oxygen Concentration.

Figure 4-15. Time to React Fuel to a Specified Depth as a Function of Temperature for a Reaction Area Equal to 10X that of Declad Fuel Using Modified Ritchie Assuming a Constant 2% Oxygen Concentration.

Figure 4-16. Gas Temperature in Rubble and Fuel Central Channels
(Time = 30 Hours).

Figure 4-17. Gas Temperature in Rubble and Fuel Exterior Channels
(Time = 30 Hours).

Figure 4-18. Gas Temperature in Rubble and Fuel Exterior Edge Channels
(Time = 30 Hours).

Figure 4-19. Temperature of Rubble Basket
(Time = 30 Hours).

Figure 4-20. Temperature of Central Elements
(Time = 30 Hours).

Figure 4-21. MCO Structure Temperatures
(Time = 30 Hours).

Figure 4-22. Oxygen Volume Fraction in Rubble and Fuel
Exterior Central Channels (Time = 30 Hours).

Figure 4-23. Oxygen Volume Fraction in Rubble and Fuel Exterior Edge Channels (Time = 30 Hours).

Figure 4-24. Gas Temperature in Rubble and Central Channels
(Time = 34 Hours).

Figure 4-25. Oxygen Volume Fraction in Rubble and Fuel Exterior Channels
(Time = 34 Hours).

Figure 4-26. Gas Temperature in Rubble and Fuel Central Channels
(Time = 40 Hours).

Figure 4-27. Gas Temperature in Rubble and Fuel Exterior Central Channels
(Time = 40 Hours).

Figure 4-28. Gas Temperature in Rubble and Fuel Exterior Edge Channels
(Time = 40 Hours).

Figure 4-29. Temperature of Rubble Basket (Time = 40 Hours).

Figure 4-30. Temperature of Central Fuel Elements (Time = 40 Hours).

Figure 4-31. MCO Structure Temperatures (Time = 40 Hours).

Figure 4-32. Oxygen Volume Fraction in Rubble and Fuel Central Channels
(Time = 40 Hours).

Figure 4-33. Oxygen Volume Fraction in Rubble and Fuel Exterior Edge Channels
(Time = 40 Hours).

Figure 4-34. Gas Temperature in Rubble and Fuel Central Channels
(Time = ~~40~~ 20 Hours).

Figure 4-35. MCO Rod and Structure Temperature for the Second Basket from the Bottom During Heat Up Using Helium for an Average Powered MCO.

Figure 4-36. MCO Rod and Structure Temperature for the Second Basket from the Bottom During Heat Up Using Argon for an Average Powered MCO.

Figure 4-37. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 0.5% by Volume.

Figure 4-38. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 1.0% by Volume.

Figure 4-39. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 1.5% by Volume.

Figure 4-40. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 2.0% by Volume.

Figure 4-41. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 3.0% by Volume.

Figure 4-42. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 4.0% by Volume.

Figure 4-43. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 5.0% by Volume.

Figure 4-44. Temperature Contour Plot for Scrap Basket, Minimum Decay Heat, Helium Purge, Porosity = 0.259, for an Inlet Oxygen Concentration of 10.0% by Volume.

Figure 4-45. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 0.5% by Volume.

Figure 4-46. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 1.0% by Volume.

Figure 4-47. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 1.5% by Volume.

Figure 4-48. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 2.0% by Volume.

Figure 4-49. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 3.0% by Volume.

Figure 4-50. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 4.0% by Volume.

Figure 4-51. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 5.0% by Volume.

Figure 4-52. Oxygen Mass Fraction Contour Plot for Scrap Basket Minimum Decay Heat Porosity = 0.259 for an Inlet Oxygen Concentration of 10.0% by Volume.

Figure 4-53. Temperature Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 0.5% by Volume.

Figure 4-54. Temperature Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 1.0% by Volume.

Figure 4-55. Oxygen Mass Fraction Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 0.5% by Volume.

Figure 4-56. Oxygen Mass Fraction Contour Plot for Scrap Basket, Maximum Decay Heat, Helium Purge, Porosity = 0.476 for an Inlet Oxygen Concentration of 1.0% by Volume.

Figure 4-57. Temperatures Versus Time During 72 Hour HCS Simulation for Various Nodes Within a Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-58. Temperatures Versus Time During Heatup Phase of HCS Simulation for Various Nodes Within a Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-59. Temperatures Versus Time During Cooldown Phase of HCS Simulation for Various Nodes Within a Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-60. Temperatures Contour Plot at 3 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-61. Temperatures Contour Plot at 6 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-62. Temperatures Contour Plot at 9 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-63. Temperatures Contour Plot at 12 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-64. Temperatures Contour Plot at 36 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-65. Temperatures Contour Plot at 60 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-66. Temperatures Contour Plot at 63 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-67. Temperatures Contour Plot at 66 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-68. Temperatures Contour Plot at 69 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-69. Temperatures Contour Plot at 72 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Argon Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-70. Temperature Versus Time During 84 Hour HCS Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-71. Temperature Versus Time During Heatup Portion of HCS Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-72. Temperature Versus Time During Cooldown Portion of HCS Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-73. Temperatures Versus Time During the Last 24 Hours of HCS Process Simulation for Various Nodes for a Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-74. Temperature Contours at 3 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-75. Temperature Contours at 6 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-76. Temperature Contours at 9 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-77. Temperature Contours at 12 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-78. Temperature Contours at 18 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-79. Temperature Contours at 24 Hours During HCS Simulation for
Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476,
No Chemical Reactions.

Figure 4-80. Temperature Contours at 30 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-81. Temperature Contours at 36 Hours During HCS Simulation for
Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476,
No Chemical Reactions.

Figure 4-82. Temperature Contours at 42 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-83. Temperature Contours at 48 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-84. Temperature Contours at 54 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-85. Temperature Contours at 60 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-86. Temperature Contours at 63 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-87. Temperature Contours at 66 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-88. Temperature Contours at 69 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-89. Temperature Contours at 72 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Helium Porosity = 0.476, No Chemical Reactions.

Figure 4-90. Temperature Contours at 75 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-91. Temperature Contours at 79 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

Figure 4-92. Temperature Contours at 81 Hours During HCS Simulation for
Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476,
No Chemical Reactions.

Figure 4-93. Temperature Contours at 84 Hours During HCS Simulation for Nominal Decay Heat Scrap Basket, Helium Purge, Porosity = 0.476, No Chemical Reactions.

5.0 CONCLUSIONS AND RECOMMENDATIONS

A series of analyses have been completed investigating the thermal-hydraulic performance and feasibility of the hot conditioning system (HCS) and process. The subject analyses used a series of one-, two-, and three-dimensional models that investigated chemical reactions, flow distributions, and combined thermal-hydraulic effects, including mass transport.

The subject analyses focus on quantifying the internal flow distributions within the multi-canister overpack (MCO), establishing the governing energy production and removal capabilities during the Hot Conditioning System (HCS) process steps, and performing process simulations for the various purge gases under consideration. The goal is to develop a series of thermal-hydraulic models that could respond to all process and safety related issues that may arise pertaining to the HCS, as well as obtain preliminary results for comparison with and verification of other analyses and provide technology-based recommendations for consideration by the HCS design authorities.

Based on efforts to develop three-dimensional models, as discussed in Chapter 3.0, the following insights are offered, which relate to the adequacy of the existing simulation capability;

1. Complex 2D and 3D modeling of the thermal or thermal-transport mechanisms require long computer run times and considerable man hours to develop the input and interpret the results. These models do not lend themselves to timely analyses considering that the thermal time constant (the time necessary to achieve 63% of a step change in temperature) could vary from 12 to 36 hours depending on the individual basket loading within the MCO and the HCS purge gas in use and the process time that must be simulated is on the order of in use five days.
2. Complex 2D modeling, or even 3D modeling of all thermal-transport mechanisms is necessary for some, but not all of the normal process or accident scenarios that must be simulated. Simple analytical models can be used for parametric analyses, provided the modeling technique chosen has been validated and verified through code-to-code comparisons at a variety of conditions.
3. Most of the important thermal-hydraulic response characteristics of the MCO, fuel baskets and HCS process simulation can be adequately described with a model capable of the following;
 - a. Thermal radiation between vertical structures
 - b. Conduction across gas gaps
 - c. Axial conduction within metal structures
 - d. Convective heat transfer with gases or liquids
 - e. Evaporation of water or the phase change from water to steam

- f. Chemical reactions, including the effects of concentration dependent reaction rate relationships.

Knowledge of the flow distribution within the MCO is necessary as a basis for design and operational decisions for the HCS dehydrating and passivation process steps. Estimates of the flow distribution within the MCO for loadings consisting of Mark Ia, Mark IV, and scrap fuel baskets were determined with the FNET hydraulic flow network program (Appendix B) and were compared to estimates obtained from a full-length MCO sub-channel COBRA-TF flow model.

The results of the flow analyses, as shown in Tables 4-1 and 4-2 indicate that the initial perforated base plate design for the Mark Ia and Mark IV fuel baskets resulted in either excessive bypass flow around the baskets or a maldistribution of flow around the fuel within a fuel basket. The optimum design would be zero bypass flow and a flow split of 59% to the inner flow channels and 41% to the outer most exterior surface of a given fuel assembly. The socketed base plate design does much better at obtaining the optimum flow splits, but still has approximately 14 to 21% bypass flow depending on the fuel type. The socketed base plate design is recommended for the Mark Ia and Mark IV fuel baskets.

The scrap basket, because of the high flow resistance associated with a porous media assumed similar to irregular shaped pieces of coal 0.75 inches in diameter, is predicted to have 46% bypass flow. With the addition of flexible flow restrictors, within the annulus between the scrap basket skirt and the MCO inner diameter, the bypass flow decreases to approximately 13 to 20% of the total MCO gas flow. Comparison of the network flow results with isothermal flow results from COBRA-TF, as shown in Table 4-3, indicated very good agreement for the socket type fuel baskets and a scrap basket with a outer perimeter flow restrictor. Bypass flow restrictors are recommended for both the scrap and fuel baskets to maximize the amount of flow passing through the various baskets, during the passivation phase, to prevent the higher oxygen concentration in the bypass flow from obscuring the true oxygen concentration as measured by the process instrumentation.

Additional design work may be required to limit flow channeling through partially or unevenly filled fuel or scrap baskets. One possible design modification for consideration involves reducing the number and spacing of the flow holes through the scrap basket baseplate. This would result in the baseplate becoming the controlling resistance rather than the porous media and would minimize flow redistribution or flow channeling within a partially or unevenly filled scrap basket. The use of dummy fuel elements to completely load out a fuel basket may be a simple solution to effectively reduce flow channeling within a partially filled fuel basket.

Based on a the results of a series of one-dimensional parametric analyses, as shown in Figures 4-7 through 4-15, the length or amount of fuel that can be passivated by a given purge flow is a function of the temperature of the fuel, the concentration of oxygen within the purge gas, and the amount of surface reaction area, and the time available to react to given depth. The reaction length (the length required to consume all of the oxygen in the purge gas flow) decreases as the temperature of the fuel and reactive surface area increases. At a fixed surface temperature, the one-dimensional calculations indicated that reaction length will increase as O_2 concentration increases.

While true for a constant axial temperature, this is misleading because the reaction rate is a function of both O_2 concentration and temperature. Therefore, in actual practice increasing O_2 concentration will increase the local reaction rate and hence the local surface temperature and will decrease reaction length. This expectation has since been confirmed through a series of three-dimensional analyses with variable oxygen concentrations by volume, which clearly show the reaction front starting at axial elevations with higher temperatures then moving down through the porous media or fuel baskets due to axial conduction and oxygen depletion. Axial conduction allows the near temperatures to increase just enough to react with oxygen and as the oxygen is depleted move toward the higher oxygen concentration (reduced reaction length). These findings are of course based on current understanding of the governing heat production and energy removal capabilities of the MCO within the HCS.

The following thermal results, conclusions, and recommendations were obtained from Section 4.4 and are based on nominal chemical reaction rate relationships associated with unirradiated and uncorroded uranium metal with oxygen, a conservative estimate of the total reactive surface area of 800000 cm^2 for each scrap basket, and the conservative assumption that the upper six inches of each fuel assembly is completely degraded. (NOTE: The above reactive surface areas are associated with the safety bases for the spent nuclear fuel project (SNFP)). The results of the thermal analyses indicate that careful consideration will need to be given to the location and variation of fuel temperatures within the MCO during the HCS passivation process to insure that:

1. Sufficient and a uniform distribution of oxygen reaches all exposed fuel surfaces such that highly reactive uranium metal is not left unpassivated in the MCO. This could occur if highly damaged fuel in the lower elevations of the MCO consume all the oxygen before it reaches the upper elevations of the MCO preventing fuel in the upper baskets from being passivated. This process may not be controllable for highly damaged fuel or scrap, since any reaction that starts will continue as oxygen continues to be added to the system or until all of the oxygen is consumed.
2. The chemical heat of reaction will be the dominate heat source at higher fuel temperatures and/or increased oxygen concentrations. This may lead to the fuel temperatures that could potentially exceed the alpha-beta phase change temperature leading to cladding failure and the extrusion of fuel into the flow channels, thereby increasing the reactive surface area many times and increasing the local reaction rate. Such a scenario may cause the fuel to melt during the passivation process step. An atmospheric ingress accident with 21% oxygen by volume will lead to a large energy spike and potentially excessive temperatures. A safety significant confinement system, a safety class confinement system, or an emergency inert gas blanketing system for the MCO, dewar flow annulus, and HCS vacuum chamber, depending on the results of a probabilistic safety analysis (PRA), may be required to mitigate the consequences of an oxygen ingress accident and allow the chemical energy to slowly dissipate.

3. The high reaction heat, coupled with low heat removal capability, may also make the process hard to control. Hot spots within the MCO will be difficult to detect by the process instrumentation given the thermal time constant of the fuel, heat transfer to adjacent fuel assemblies or MCO structures, and the potential for significant oxygen bypass.
4. The presence of radial and axial temperature profiles in the fuel during passivation are likely to result in non-uniform oxygen consumption which will result in local hot spots.

Other findings are summarized as follows:

1. The use of helium, rather than argon, as the HCS process purge gas can significantly reduce the heatup and cooldown times and is recommended as the purge gas of choice for the HCS process. Leakage and cost considerations may limit the effectiveness of this option. It is also recommended that a helium recycle system be investigated.

The proposed 12 hour HCS cooldown is not adequate for either argon or helium. Significant temperature gradients exist within the MCO, especially during the 12 hour HCS cooldown period prior to commencing the passivation phase. (Helium will minimize, but not completely eliminate temperature gradients.) These gradients could result in local temperatures sufficiently high enough to produce a chemically reactive hot spot given the oxygen feed during the passivation phase.

A minimum of a 12 hour extension beyond the 12 hour HCS cooldown period, while holding at an inlet temperature of 423.16 °F (302 °F), appears to provide an adequate time given helium as the purge gas to minimize the temperature gradients within the scrap basket prior to commencing the passivation phase. A hold time longer than 12 hours will be required for fuel baskets, given that the effective thermal resistance of the scrap basket is less than the fuel baskets, but has not yet been investigated. (Much longer hold times will be required for argon under any condition.) Any modification to the proposed HCS process times must be adequately investigated for thermal impacts on both the scrap and fuel baskets.

2. The presence of two scrap baskets (top and bottom) within an MCO leads to a set of unique thermal concerns. These are;
 - a. At the proposed inlet temperature of 150 °C (302 °F) the lower scrap basket will consume all the oxygen within the first few inches resulting in excessive temperatures (> 1000 °F). Reducing the inlet temperature by 50 °C allows oxygen to pass through the lower scrap basket to higher levels, but the increase in purge gas temperature as it reaches the upper scrap basket, produces the same temperature excursions as in the lower basket.
 - b. A single chemically active "hot spot" within the scrap or fuel baskets will eventually lead to excessive temperatures. A "hot

and cold spot" analysis given statistical variations in the decay heat, reactive surface areas, the geometrical area-to-volume ratio, and scrap basket local porosity has not yet been initiated.

- c. Currently planned process instrumentation may not be able determine if the oxygen is being consumed on an distributed or localized "hot spot" basis. The purge gas flow from the MCO, as measured by the process instrumentation, could have a significant oxygen concentration due to sufficient bypass flow around the scrap and socketed fuel basket designs, while the remainder of the oxygen has been consumed in a very local area producing excessive fuel temperatures. It will be difficult to detect such local hot spots. As previously recommended, bypass flow should be minimized by using flow restrictors on both the scrap and fuel baskets. Other possible designs to minimize bypass flow include full length skirts that will intersect with each tier and a seal ring around the upper perimeter of the lower spider assembly.
 - d. The process instrumentation may not be adequate to detect the increase in purge gas temperature associated with a "hot spot", due to the long thermal time constant of the fuel or heat transfer to adjacent fuel and/or MCO internals.
3. A single upper scrap basket is recommended.
 4. Given the potential variability in MCO contents, the HCS process operational strategies should be designed to allow for variable (0 - 5%) rather than a constant oxygen concentration and a variable helium purge gas flow rate (to be determined) that would help to minimize the radial and axial temperature gradients.
 5. The above conclusions and recommendations assume conservative reactive surface areas and published reaction rate relationships based on unirradiated and uncorroded uranium metal. Characterization data based on actual K Basin fuel is needed in these areas.

In summary, a uniform distribution of oxygen will be hard to achieve. Chemically active "hot spots" leading to excessive temperatures can occur via local variations in reactive surface area, temperature gradients, and oxygen concentrations. Additional model development and analyses are recommended to investigate combinations of scrap and fuel baskets within a MCO; such as, a less than the full complement of baskets, or a single upper or lower scrap and four fuel baskets, or five fuel and no scrap baskets. The following analyses are strongly recommended: (1) investigate the effects of decreased reactive surface areas, reaction rate relationships based on actual characterization data, variable process flow rates, a variable oxygen concentration feed during the passivation phase, and vacuum conditions, (2) investigate the effects of "statistical" based non-uniform distributions for decay heat, reactive surface areas, and scrap basket porosity, and (3) determine a modified HCS process heatup and/or cooldown rate, that could, respectively, in the minimum amount of time, obtain the minimum temperature necessary for complete dehydriding and reduce the temperature gradients within the MCO prior to commencing the

passivation phase. Items #1 and #2 must be performed to support the safety analysis report (SAR) and the final HCS design. (Item #2 is especially important when investigating the effects of chemically active "hot and cold spots" given a more realistic treatment of the variations expected with actual MCO loadings.) Item #3 must be performed to support HCS process operations given a final design or the assumed "statistical" variations in MCO loadings.

6.0 REFERENCES

- Internal Memo, T. R. Beaver to C. R. Miska, "Flow Distribution Within the SNF Storage Scrap Basket," 74A50-96-TRB-015, dated May 6, 1996.
- Internal Memo, T. R. Beaver to C. R. Miska, "Results of Scoping Calculations to Determine Internal MCO Flow Splits for Various Mark IA and Mark IV Basket Designs," 74A50-96-TRB-011, dated March 27, 1996.
- Cooper, T. D., 1996a, *Recommended Rate Constants for Corrosion of N Reactor Fuel*, WHC-SD-SNFTI-020, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Cooper, T. D., 1996b, *Hydrogen from Hydride*, (cc:Mail to F. J. Heard, March 31, 1996, attached as Appendix C), Westinghouse Hanford Company, Richland, Washington.
- Heard, F. J., 1996, Thermal Hydraulic Feasibility Assessment for the Spent Nuclear Fuel Project, WHC-SD-WM-ER-525, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Heard, F. J., 1994, *FIDAP Version 7.06 - Validation/Verification*, WHC-SD-WM-ER-302, Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Idelchik, I. E., 1986, "Handbook of Hydraulic Resistance," Second Edition, Springer-Verlag, New York, New York.
- Kavinay, M., 1995, "Principles of Heat Transfer in Porous Media," Second Edition, Springer-Verlag, New York, New York.
- Lawrence, L. A., 1995, *Data Quality Objectives for the Reaction Kinetic Studies of K West Fuel Samples*, WHC-SD-SNF-DQO-007, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- McAdams, W. H., 1954, *Heat Transmission*, 3rd Ed., McGraw-Hill Book Company, New York, New York.
- NRC-1985, *Analysis of Flecht-Seaset 163-Rod Blocked Bundle Data Using COBRA-TF*, NUREG/CR-4166, United States Nuclear Regulatory Commission, Washington, D. C.
- Pearce, R. J., 1989, *A Review of the Rates of Reaction of Unirradiated Uranium Gaseous Atmospheres*, RD/B/6231/R89, Central Electricity Generating Board, Berkeley Nuclear Laboratories, United Kingdom.
- Ritchie, A. G., 1981, "A Review of the Rates of Reactions for Uranium in Oxygen and Water Vapor at Temperatures up to 300 °C," *Journal of Nuclear Materials*, 102, pp 170-182.
- Short, S. M., and M. M. Beary, 1995, *SNF Project Technical Databook*, WHC-SD-SNF-TI-015, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

Willis, W. L. and A. N. Praga, 1995, *105-K Basin Material Design Basis Feed Description for Spent Nuclear Fuel Project Facilities*, WHC-SD-SNF-TI-009, Westinghouse Hanford Company, Richland, Washington.

APPENDIX A. FORTRAN LISTING OF EFFECTIVE THERMAL CONDUCTIVITY PROGRAM.

```

PROGRAM KEFF
C This program calculates the effective thermal conductivity of
C a porous media using Hadley's correlation for conduction and
C equation 5.304 from Kaviany's book for thermal radiation.
C
      OPEN(7,FILE='kinput')
      OPEN(8,FILE='ke.out')
C
C Get the porosity for the porous media
      PRINT*, 'Input the porosity '
      READ (5,*) P
C Specify the gas species for the continuous phase (J=1, helium; J=2, argon;
C J=3, nitrogen)
      PRINT*, 'Input gas species; 1=helium, 2=argon, 3= nitrogen '
      READ (5,*) J
C Get the mean particle diameter (In)
      PRINT*, 'Input mean particle diameter (In) '
      READ (5,*) Dp
C Get the solid phase emissivity
      PRINT*, 'Input emissivity of solid phase '
      READ (5,*) EMS
C
      PRINT*, 'Enter 1 if British units, 2 if SI '
      READ (5,*) ITYPE
C
      IF(ITYPE .EQ. 1) THEN
        WRITE(8,2) P, J, EMS, Dp
      ELSE
        WRITE(8,3) P, J, EMS, Dp
      END IF
C Read in the material properties of the porous media and
C continuous phase as a function of temperature
      CALL INPUT
C
C Note: material properties are in SI units.
C Convert particle diameter to feet.
      Dp = Dp/12.0
C ***** Deg. F or Deg. K *****
      IF(ITYPE .EQ. 1) THEN
        TT = 50.0
      ELSE
        T = 300.0
      END IF
C *****
      DO 100 I = 1,36
C Convert Deg. F to Deg. K, Tables are in Deg. K
      IF(ITYPE .EQ. 1) T = (TT-32.0)/1.8+273.15
C
      CALL TABLE(T,'XKUN ',XKUN)
      IF(J .EQ.1) THEN
        CALL TABLE(T,'XKHE ',XKHE)

```

```

      SF = XKUN/XKHE
      XF = XKHE
    ELSE IF(J.EQ. 2) THEN
      CALL TABLE(T,'XKAR ',XKAR)
      SF = XKUN/XKAR
      XF = XKAR
    ELSE
      CALL TABLE(T,'XKN2 ',XKN2)
      SF = XKUN/XKN2
      XF = XKN2
    END IF
  C Calculate conduction component using Hadley's equation
      IF(P.LE. 0.298) THEN
        FN = -0.405-3.15*(P-0.0827)
      ELSE
        FN = -1.084-6.778*(P-0.298)
      END IF
      ALPHA = 10**FN
      FO = 0.8+0.1*P
      EF = (1.0-ALPHA)*(P*FO+SF*(1.0-P*FO))/(1.0-P*(1.0-FO)+SF*P*
1      (1.0-FO))+ALPHA*(2.0*SF**2*(1.0-P)+SF*(1.0+2.0*P))/
2      (SF*(2.0+P)+1.0-P)
  C ***** BTU/HR/FT/F or w/m/k *****
      IF(ITYPE.EQ. 1) THEN
        XKC = 0.5782*XF*EF
      ELSE
        XKC = XF*EF
      END IF
  C *****
  C Calculate radiation component assuming 1-dim. plane geometry
  C Convert Deg. K to Deg. F
      IF(ITYPE.NE. 1) TT = 1.8*(T-273.15)+32.0
  C
      TM3 = (TT+460.0)**3
      SIGMAT = 1.714E-9*TM3
      XKS = 0.5782*XKUN/(4.0*Dp*SIGMAT)
      FAC = 1.5353*XKS**0.8011/EMS
      FF = 0.5756*EMS*ATAN(FAC)+0.1843
      IF(ITYPE.EQ. 1) THEN
        XKR = 4.0*FF*Dp*SIGMAT
      ELSE
        XKR = (4.0*FF*Dp*SIGMAT)/0.5782
      END IF
  C Calculate the combined effective conductivity
      XKE = XKC+XKR
  C
  C ***** Write the results and increment temperatures *****
      IF(ITYPE.EQ. 1) THEN
        WRITE(8,1) TT, XKC, XKR, XKE
        TT = TT+50.0
      ELSE
        WRITE(8,1) T, XKC, XKR, XKE
        T = T+25.0
      END IF

```

```

C *****
100 CONTINUE
1  FORMAT(2X,F7.1,5X,F10.4,5X,F10.4,5X,F10.4)
C
2  FORMAT(5X'Effective conductivity versus temperature for P=',F6.4,
1  ', gas type',I3,', Emissivity =',F5.2,'% Dia. =',F5.2,'In.'/
2  10x,'Col.1 - T, Col.2 - Conduction, Col.3 - Radiation, Col.4 - Co
3  mbined'/5X,'T - Deg.F, K - BTU/hr-Ft-F; 1 = He gas, 2 = Argon
4  gas, 3 = Nitrogen gas')
3  FORMAT(5X'Effective conductivity versus temperature for P=',F6.4,
1  ', gas type',I3,', Emissivity =',F5.2,'% Dia. =',F5.2,'In.'/
2  10x,'Col.1 - T, Col.2 - Conduction, Col.3 - Radiation, Col.4 - Co
3  mbined'/5X,'T - Deg.K, K - Watt/m-Deg.K 1 = He gas, 2 = Argon
4  gas, 3 = Nitrogen gas')
C *****
END
SUBROUTINE INPUT
C***
C*** SUBROUTINE TO PROVIDE INPUT DATA TO CALCULATE EFFECTIVE THERMAL
C*** CONDUCTIVITY IN POROUS MEDIA
C***
DIMENSION TEMP(100), XKUN(100), XKHE(100), XKAR(100), XKN2(100)
CHARACTER*5 VAR, VAR1, VAR2, VAR3, VAR4
CHARACTER*1 LINE1(80), LINE2(80)
DATA VAR1/'XKUN ',VAR2/'XKHE ',VAR3/'XKAR ',VAR4/'XKN2 '/
READ (7,1100) (LINE1(I),I = 1,80)
READ (7,1100) (LINE2(I),I = 1,80)
NN = 1
300 READ(7,*,END=600,Iostat=IOS) TEMP(NN),XKUN(NN),XKHE(NN),
1  XKAR(NN),XKN2(NN)
NN = NN + 1
GO TO 300
600 CONTINUE
NDC = NN-1
RETURN
ENTRY TABLE (T,VAR,ARG)
C***
C*** FIND THE DATA INTERVAL IN WHICH T LIES
C***
CALL HUNT(TEMP,NDC,T,LO)
IF(LO .EQ. 0) LO=1
RAT1 = (T - TEMP(LO))/(TEMP(LO+1) - TEMP(LO))
IF (VAR .EQ. VAR1) THEN
ARG = XKUN (LO) + RAT1 * (XKUN (LO+1) - XKUN (LO))
ELSE IF (VAR .EQ. VAR2) THEN
ARG = XKHE (LO) + RAT1 * (XKHE (LO+1) - XKHE (LO))
ELSE IF (VAR .EQ. VAR3) THEN
ARG = XKAR (LO) + RAT1 * (XKAR (LO+1) - XKAR (LO))
ELSE IF (VAR .EQ. VAR4) THEN
ARG = XKN2 (LO) + RAT1 * (XKN2 (LO+1) - XKN2 (LO))
ELSE
PRINT *, ' NOT A VALID ENTRY FOR TABLE LOOKUP ',VAR
ARG = 0.0
END IF

```

```

      RETURN
1100  FORMAT (80A1)
1200  FORMAT (' ',80A1)
1300  FORMAT (5X,G10.3,2X,G10.3,2X,G10.3,2X,G10.3,2X,G10.3)
      END
      SUBROUTINE HUNT(XX,N,X,JLO)
C   Given an array XX of length N, and given a value X, returns a value JLO
C   such that X is between XX(JLO) and XX(JLO+1). XX must be monotonic,
C   either increasing or decreasing. JLO=0 or JLO=N is returned to indicate
C   that X is out of range. JLO on input is taken as the initial guess for
C   JLO on output.
      DIMENSION XX(N)
      LOGICAL ASCND
      ASCND=XX(N).GT.XX(1)
      IF(JLO.LE.0.OR.JLO.GT.N)THEN
        JLO=0
        JHI=N+1
        GO TO 3
      ENDIF
      INC=1
      IF(X.GE.XX(JLO).EQV.ASCND)THEN
1      JHI=JLO+INC
        IF(JHI.GT.N)THEN
          JHI=N+1
        ELSE IF(X.GE.XX(JHI).EQV.ASCND)THEN
          JLO=JHI
          INC=INC+INC
          GO TO 1
        ENDIF
      ELSE
2      JHI=JLO
        JLO=JHI-INC
        IF(JLO.LT.1)THEN
          JLO=0
        ELSE IF(X.LT.XX(JLO).EQV.ASCND)THEN
          JHI=JLO
          INC=INC+INC
          GO TO 2
        ENDIF
      ENDIF
3      IF(JHI-JLO.EQ.1)RETURN
      JM=(JHI+JLO)/2
      IF(X.GT.XX(JM).EQV.ASCND)THEN
        JLO=JM
      ELSE
        JHI=JM
      ENDIF
      GO TO 3
      END

```

Thermal conductivity versus temperature for Uranium, Helium, Argon and Nitrogen. Temperature - Deg. K, Conductivity - W/m-K

270.	26.9	0.1405	0.01619	0.02374
300.	27.0	0.1499	0.01772	0.02589
370	27.0	0.1708	0.02103	0.03065
470.	29.0	0.2013	0.0252	0.0369
570.	31.0	0.236	0.0291	0.0426
670.	33.0	0.269	0.0326	0.0478
770.	35.0	0.298	0.0359	0.0527
870.	38.0	0.326	0.0390	0.0574
920.	39.0	0.34	0.0404	0.0596
940.	39.1	0.346	0.0410	0.0605
970.	40.0	0.354	0.0419	0.0618
1020.	41.0	0.359	0.0433	0.0639
1050.	41.6	0.376	0.0441	0.0651
1070.	42.3	0.381	0.0446	0.0659
1120.	43.4	0.394	0.0460	0.0680
1170.	44.6	0.408	0.0473	0.0701
1200.	45.3	0.416	0.0481	0.0713
1250.	46.5	0.430	0.0495	0.0733

APPENDIX B. FORTRAN LISTING OF HYDRAULIC NETWORK PROGRAM.

```

PROGRAM FNET
C
C MCO assembly with MARK IV Fuel in Socket type fuel assembly baskets
C (54 elements/basket). Baskets #1 and #5 are filled with rubble and
C possibly some vertically aligned outer fuel elements. Seals on both lower
C and upper rubble baskets. Laminar flow friction loss assumes 64/Re.
C Calculations include hydraulic head. Rubble baskets have perforated
C plate bottom with 1/4 inch holes.
C
C ***** INPUT PARAMETERS *****
C NARA ----- Number of pressure nodes in model
C NSARA ----- Number of interconnecting piping segments
C NNX ----- Number of fixed pressures
C NX(i) ----- Node number of each specified pressure
C PN(i) ----- Fixed pressure value corresponding to each NX(i)
C NNW ----- Node number of source or sink flowrate
C W(i) ----- Fixed source (+) or sink (-) flowrate at node NNW
C ***** CODE PARAMETERS *****
C GP(i,j) ----- Flow admittance array, GP(i,j)=1.0/R(i,j)
C C(i,j) ----- Hydraulic head array, C(i,j)=Rho*G(i,j)*(Hj-Hi)
C P(i) ----- Pressure array
C MDOTI(i) ----- Initial or new segment(i) flowrate
C MDOTO(i) ----- Old segment(i) flowrate from previous iteration
C RHOr ----- Reference density for converting mass flow to SCFM
C WF ----- Weighing function for flowrate iterations
C EPSN ----- Normalized convergence criteria
C
C   PARAMETER (NARA=8, NSARA=9)
C   IMPLICIT REAL*8(A-H,O-Z)
C   REAL*8 MDOT, MDOTI, MDOTO, M1(7), M2(7), M3(7), M4(7), NF
C   DIMENSION
C   $   C(NARA,NARA),   GP(NARA,NARA),   P(NARA),   MDOTI(NSARA),
C   $   MDOTO(NSARA),   II(NSARA),   JJ(NSARA),   DMDOT(NSARA),
C   $   PN(20),   NX(20),   SCFM(NSARA),   W(NARA),
C   $   G(NARA,NARA),   D(NARA),   PIW(NARA)
C   COMMON /SOLV/ NN,NX,NNX,PNX
C
C
C   PIPING FRICTION FACTOR
C   FFAC(ED,Z) = (1.0/(-2.0*DLOG10(ED/3.7-5.02/Z*DLOG10(ED/3.7+
C   1   13.0/Z))))**2
C
C   DENSITY (LBM/FT**3)
C   RHOA(PP,Z) = 144.0*PP/(53.35*(Z+459.7))
C   RHOAR(PP,Z) = 144.0*PP/(38.6*(Z+459.7))
C
C   VISCOSITY (LBM/FT/SEC)
C   AMUA(Z) = 1.095E-5+Z*(1.813E-8-Z*(4.375E-12))
C   AMUAR(Z) = 1.4084E-5+Z*(1.9974E-8-2.6278E-12*Z)
C   AMUHE(Z) = 1.2256E-5+Z*(1.5803E-8-1.6841E-12*Z)

```

```

C Piping segment definitions in terms of the terminating nodes .
C Segment I is terminated by nodes II and JJ.
  DATA (II(I),I=1,NSARA)/ 1, 1, 2, 3, 4, 5, 6, 7, 2/
  DATA (JJ(I),I=1,NSARA)/ 7, 2, 3, 4, 5, 6, 8, 8, 7/
C
  OPEN(8, FILE='fnet.out')
C
C Read input
C
  NNX = 2
  NX(1) = 1
  NX(2) = 8
C
C PRINT *, ' INPUT TOTAL NUMBER OF SPECIFIED PRESSURES '
C READ (5,*) NNX
C PRINT*, ' INPUT NODE NUMBER OF EACH SPECIFIED PRESSURE '
C READ (5,*) (NX(I), I=1,NNX)
C PRINT*, ' INPUT PRESSURE (psia) CORRESPONDING TO EACH NODE NUMBER '
  READ (5,*) (PNX(I), I=1,NNX)
C PRINT*, ' INPUT NUMBER OF FUEL ELEMENTS IN RUBBLE BASKET '
  READ (5,*) NF
C PRINT*, ' INPUT PLATE POROSITY '
  READ (5,*) PPor
C
C Write input to output file
C
C OUTPUT TOTAL NUMBER OF SPECIFIED PRESSURES
  WRITE (8,*) NNX
C OUTPUT NODE NUMBER OF EACH SPECIFIED PRESSURE
  WRITE (8,*) (NX(I), I=1,NNX)
C OUTPUT PRESSURE (psia) CORRESPONDING TO EACH NODE NUMBER '
  WRITE (8,*) (PNX(I), I=1,NNX)
  WRITE (8,*) PPor
C
C Program constants
C
  WF = 0.1
  N = NARA
  NSEG = NSARA
  NODES = NARA
  NNMI = NODES-1
  NNW = 50
  NN = N-NNX
  FLOW = 0.0
  EPSN = 1.0E-5
  TEMP = 428.0
  Gc = 32.2
  RHOr = 0.1055
  Por = 0.46
  Dgr = 0.0625
  Ht = 2.0833
  Xk = 1.53/Por**4.2
  Zetaq = 1.246785*PPor**(-2.249755)
C

```

```

C  INITIAL CALCULATIONS
C
C  INITIALIZE SOURCE/SINK FLOWS AND NODAL PRESSURES
C  FLOWRATE IS IN LB/SEC. AND PRESSURE IS IN PSIA
      DO 10 I=1,N
        W(I) = 0.0
        P(I) = PNK(1)
        IF(I .EQ. NNW) W(I)=FLOW
10    CONTINUE
C
C  INITIAL GUESS FOR PIPING SEGMENT MASS FLOWS (lb/sec)
      DO 15 I=1,NSARA
        MDOTI(I) = 0.05
15    CONTINUE
C
C  MAIN CALCULATION LOOP
C
C  CALCULATE NEW NODAL PRESSURES (lb/in**2) AND SYSTEM FLOWRATES
C  FOR NEW PRESSURE BOUNDARY CONDITIONS AT THE PRESENT ITERATION STEP
C
      ICOUNT = 0
20    CONTINUE
      ICOUNT = ICOUNT+1
C
C  DETERMINE FLOW ADMITTANCES GP(i,j) FOR THE VARIOUS FLOW PATHS THROUGH
C  THE PIPING NETWORK.
C
C  LINE SEGMENT 1; (Node 1 to Node 7), Flow between guide cone and
C                      central flow tube
      Ac = 0.00118
      Dc = 0.01
      E = 0.004
      MDOT = ABS(MDOTI(1))
      PBAR = 0.5*(P(1)+P(7))
      RHO = RHOAR(PBAR,TEMP)
      RE = MDOT*Dc/(Ac*AMUAR(TEMP))
      FL = 64.0/(RE+0.0001)
      IF(RE .LT. 100.0) THEN
        FT = 0.0
      ELSE
        FT = FFAC(E,RE)
      END IF
      FF = DMAX1(FL,FT)
      R = (8.33*FF+1.50)*MDOT/(64.4*Ac**2*144.0*RHO)
      GP(1,7) = 1.0/R
      GP(7,1) = GP(1,7)
      C(1,7) = RHO*0.4167/R
      C(7,1) = -C(1,7)
C  LINE SEGMENT 2; (Node 1 to Node 2), Flow through bottom strainer
      A2 = 0.0491
      MDOT = ABS(MDOTI(2))
      PBAR = 0.5*(P(1)+P(2))
      RHO = RHOAR(PBAR,TEMP)
      R = 2.5*MDOT/(64.4*A2**2*144.0*RHO)

```



```

GP(1,2) = 1.0/R
GP(2,1) = GP(1,2)
C(1,2) = RHO*0.4167/R
C(2,1) = -C(1,2)
C LINE SEGMENT 3; (Node 2 to Node 3), Flow through Basket #1 (Rubble basket)
  IF(ICOUNT .EQ. 1) THEN
    M1(3) = MDOTI(3)
    M2(3) = MDOTI(3)
    M3(3) = MDOTI(3)
    M4(3) = MDOTI(3)
  ELSE
    M1(3) = ABS(R1/R11*MDOTI(3))
    M2(3) = 0.0
    M3(3) = ABS(R1/R13*MDOTI(3))
    M4(3) = ABS(R1/R14*MDOTI(3))
  END IF
C Flow through rubble in basket
  Af = 2.7917-0.0321*NF
  PBAR = 0.5*(P(2)+P(3))
  RHO = RHOAR(PBAR,TEMP)
  RE = 0.45*M1(3)*Dgr/((1.0-Por)*DSQRT(Por)*Af*AMUAR(TEMP))
  FF = 75.0/RE+15.0/DSQRT(RE)+1.0
  Xn = Xk*FF*Ht/Dgr
C plate bottom below rubble
  REp = 0.0208*M1(3)/(Af*AMUAR(TEMP))
  EPRE = 0.231614*REp**(0.119679)
  Zeta = 33.0/(REp*PPor**2)+EPRE*Zetaq
  R11 = (Xn+Zeta)*M1(3)/(64.4*Af**2*144.0*RHO)
C Flow through the fuel outer element only
  IF(NF .GT. 0.0) THEN
    Aa = 0.01578*NF
    Da = 0.14175
    E = 0.002
    RE = M3(3)*Da/(Aa*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
C plate bottom below fuel element
    REp = 0.0208*M3(3)/(Aa*AMUAR(TEMP))
    EPRE = 0.231614*REp**(0.119679)
    Zeta = 33.0/(REp*PPor**2)+EPRE*Zetaq
    R13 = (15.34*FF+Zeta)*M3(3)/(64.4*Aa**2*144.0*RHO)
  ELSE
    R13 = 1.0E20
  END IF
C Flow bypass between basket and MCO
  AB = 0.0931
  DB = 0.0312
  E = 0.004
  RE = M4(3)*DB/(AB*AMUAR(TEMP))

```

```

FL = 64.0/(RE+0.0001)
IF(RE .LT. 100.0) THEN
  FT = 0.0
ELSE
  FT = FFAC(E,RE)
END IF
FF = DMAX1(FL,FT)
C basket mechanical seal
EPRE = 0.231614*RE**(0.119679)
Zetat = 6.13296*re**(-0.48622)
Zeta = 2.0*(8.3483*Zetat+10.06*EPRE)
R14 = (71.79*FF+Zeta)*M4(3)/(64.4*AB**2*144.0*RHO)
C Equivalent resistance coefficient
R1 = 1.0/(1.0/R11+1.0/R13+1.0/R14)
GP(2,3) = 1.0/R1
GP(3,2) = GP(2,3)
C(2,3) = RHO*2.2375/R1
C(3,2) = -C(2,3)
C LINE SEGMENT 4; (Node 3 to Node 4), Flow through Basket #2 (Socket Type)
IF(ICOUNT .EQ. 1) THEN
  M1(4) = MDOTI(4)
  M2(4) = MDOTI(4)
  M3(4) = MDOTI(4)
  M4(4) = MDOTI(4)
ELSE
  M1(4) = ABS(R2/R21*MDOTI(4))
  M2(4) = ABS(R2/R22*MDOTI(4))
  M3(4) = ABS(R2/R23*MDOTI(4))
  M4(4) = ABS(R2/R24*MDOTI(4))
END IF
C Flow through fuel element centers
AI = 54.0*0.00125
DI = 0.03992
E = 0.0
PBAR = 0.5*(P(3)+P(4))
RHO = RHOAR(PBAR,TEMP)
RE = M1(4)*DI/(AI*AMUAR(TEMP))
FL = 64.0/(RE+0.0001)
IF(RE .LT. 100.0) THEN
  FT = 0.0
ELSE
  FT = FFAC(E,RE)
END IF
FF = DMAX1(FL,FT)
R21 = (54.36*FF+1.5)*M1(4)/(64.4*AI**2*144.0*RHO)
C Flow through fuel element annuli
An = 54.0*0.00686
Dn = 0.03517
E = 0.0
RE = M2(4)*Dn/(An*AMUAR(TEMP))
FL = 64.0/(RE+0.0001)
IF(RE .LT. 100.0) THEN
  FT = 0.0
ELSE

```

```

      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R22 = (61.85*FF+1.5)*M2(4)/(64.4*An**2*144.0*RHO)
C Flow external to fuel elements
    AE = 54.0*4.231E-3
    Af = 0.9658
    DE = 0.01292
    Df = 0.0899
    E = 0.004
    RE = M3(4)*DE/(AE*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    Fe = DMAX1(FL,FT)
    RE = M3(4)*Df/(Af*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R23 = ((16.96*Fe+1.5)/AE**2+24.19*FF/Af**2)*M3(4)/(64.4*144.0*RHO)
C Flow bypass between basket and MCO
    AB = 0.09332
    DB = 0.0313
    E = 0.004
    RE = M4(4)*DB/(AB*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R24 = (37.3*FF+1.5)*M4(4)/(64.4*AB**2*144.0*RHO)
C Equivalent resistance coefficient
    R2 = 1.0/(1.0/R21+1.0/R22+1.0/R23+1.0/R24)
    GP(3,4) = 1.0/R2
    GP(4,3) = GP(3,4)
    C(3,4) = RHO*2.2375/R2
    C(4,3) = -C(3,4)
C LINE SEGMENT 5; (Node 4 to Node 5), Flow through Basket #3 (Socket Type)
    IF(ICOUNT .EQ. 1) THEN
      M1(5) = MDOTI(5)
      M2(5) = MDOTI(5)
      M3(5) = MDOTI(5)
      M4(5) = MDOTI(5)
    ELSE
      M1(5) = ABS(R3/R31*MDOTI(5))

```

```

      M2(5) = ABS(R3/R32*MDOTI(5))
      M3(5) = ABS(R3/R33*MDOTI(5))
      M4(5) = ABS(R3/R34*MDOTI(5))
    END IF
  C Flow through fuel element centers
  AI = 54.0*0.00125
  DI = 0.03992
  E = 0.0
  PBAR = 0.5*(P(4)+P(5))
  RHO = RHOAR(PBAR,TEMP)
  RE = M1(5)*DI/(AI*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  FF = DMAX1(FL,FT)
  R31 = (54.36*FF+1.5)*M1(5)/(64.4*AI**2*144.0*RHO)
  C Flow through fuel element annuli
  An = 54.0*0.00686
  Dn = 0.03517
  E = 0.0
  RE = M2(5)*Dn/(An*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  FF = DMAX1(FL,FT)
  R32 = (61.85*FF+1.5)*M2(5)/(64.4*An**2*144.0*RHO)
  C Flow external to fuel elements
  AE = 54.0*4.231E-3
  Af = 0.9658
  DE = 0.01292
  Df = 0.0899
  E = 0.004
  RE = M3(5)*DE/(AE*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  Fe = DMAX1(FL,FT)
  RE = M3(5)*Df/(Af*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  FF = DMAX1(FL,FT)

```

```

      R33 = ((16.96*Fe+1.5)/AE**2+24.19*FF/AF**2)*M3(5)/(64.4*144.0*RHO)
C Flow bypass between basket and MCO
  AB = 0.09332
  DB = 0.0313
  E = 0.004
  RE = M4(5)*DB/(AB*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  FF = DMAX1(FL,FT)
  R34 = (37.3*FF+1.5)*M4(5)/(64.4*AB**2*144.0*RHO)
C Equivalent resistance coefficient
  R3 = 1.0/(1.0/R31+1.0/R32+1.0/R33+1.0/R34)
  GP(4,5) = 1.0/R3
  GP(5,4) = GP(4,5)
  C(4,5) = RHO*2.2375/R3
  C(5,4) = -C(4,5)
C LINE SEGMENT 6; (Node 5 to Node 6), Flow through Basket #4 (Socket Type)
  IF(ICOUNT .EQ. 1) THEN
    M1(6) = MDOTI(6)
    M2(6) = MDOTI(6)
    M3(6) = MDOTI(6)
    M4(6) = MDOTI(6)
  ELSE
    M1(6) = ABS(R4/R41*MDOTI(6))
    M2(6) = ABS(R4/R42*MDOTI(6))
    M3(6) = ABS(R4/R43*MDOTI(6))
    M4(6) = ABS(R4/R44*MDOTI(6))
  END IF
C Flow through fuel element centers
  AI = 54.0*0.00125
  DI = 0.03992
  E = 0.0
  PBAR = 0.5*(P(5)+P(6))
  RHO = RHOAR(PBAR,TEMP)
  RE = M1(6)*DI/(AI*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  FF = DMAX1(FL,FT)
  R41 = (54.36*FF+1.5)*M1(6)/(64.4*AI**2*144.0*RHO)
C Flow through fuel element annuli
  An = 54.0*0.00686
  Dn = 0.03517
  E = 0.0
  RE = M2(6)*Dn/(An*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE .LT. 100.0) THEN

```

```

      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R42 = (61.85*FF+1.5)*M2(6)/(64.4*An**2*144.0*RHO)
  C Flow external to fuel elements
    AE = 54.0*4.231E-3
    Af = 0.9658
    DE = 0.01292
    Df = 0.0899
    E = 0.004
    RE = M3(6)*DE/(AE*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    Fe = DMAX1(FL,FT)
    RE = M3(6)*Df/(Af*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R43 = ((16.96*Fe+1.5)/AE**2+24.19*FF/Af**2)*M3(6)/(64.4*144.0*RHO)
  C Flow bypass between basket and MCO
    AB = 0.09332
    DB = 0.0313
    E = 0.004
    RE = M4(6)*DB/(AB*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
      FT = 0.0
    ELSE
      FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R44 = (37.3*FF+1.5)*M4(6)/(64.4*AB**2*144.0*RHO)
  C Equivalent resistance coefficient
    R4 = 1.0/(1.0/R41+1.0/R42+1.0/R43+1.0/R44)
    GP(5,6) = 1.0/R4
    GP(6,5) = GP(5,6)
    C(5,6) = RHO*2.2375/R4
    C(6,5) = -C(5,6)
  C LINE SEGMENT 7; (Node 6 to Node 8), Flow through Basket #5 (Rubble basket)
    IF(ICOUNT .EQ. 1) THEN
      M1(7) = MDOTI(7)
      M2(7) = MDOTI(7)
      M3(7) = MDOTI(7)
      M4(7) = MDOTI(7)

```

```

ELSE
  M1(7) = ABS(R5/R51*MDOTI(7))
  M2(7) = 0.0
  M3(7) = ABS(R5/R53*MDOTI(7))
  M4(7) = ABS(R5/R54*MDOTI(7))
END IF
C Flow through rubble in basket
Af = 2.7917-0.0321*NF
PBAR = 0.5*(P(6)+P(8))
RHO = RHOAR(PBAR,TEMP)
RE = 0.45*M1(7)*Dgr/((1.0-Por)*DSQRT(Por)*Af*AMUAR(TEMP))
FF = 75.0/RE+15.0/DSQRT(RE)+1.0
Xn = Xk*FF*Ht/Dgr
C bottom plate
REp = 0.0208*M1(7)/(Af*AMUAR(TEMP))
EPRE = 0.231614*REp**(0.119679)
Zeta = 33.0/(REp*PPor**2)+EPRE*Zetaq
R51 = (Xn+Zeta)*M1(7)/(64.4*Af**2*144.0*RHO)
C Flow through the fuel element outer element only
IF(NF.GT. 0.0) THEN
  Aa = 0.01578*NF
  Da = 0.14175
  E = 0.002
  RE = M3(7)*Da/(Aa*AMUAR(TEMP))
  FL = 64.0/(RE+0.0001)
  IF(RE.LT. 100.0) THEN
    FT = 0.0
  ELSE
    FT = FFAC(E,RE)
  END IF
  FF = DMAX1(FL,FT)
C bottom plate
  REp = 0.0208*M3(7)/(Aa*AMUAR(TEMP))
  EPRE = 0.231614*REp**(0.119679)
  Zeta = 33.0/(REp*PPor**2)+EPRE*Zetaq
  R53 = (15.34*FF+Zeta)*M3(7)/(64.4*Aa**2*144.0*RHO)
ELSE
  R53 = 1.0E20
END IF
C Flow bypass between basket and MCO
AB = 0.0931
DB = 0.0312
E = 0.004
RE = M4(7)*DB/(AB*AMUAR(TEMP))
FL = 64.0/(RE+0.0001)
IF(RE.LT. 100.0) THEN
  FT = 0.0
ELSE
  FT = FFAC(E,RE)
END IF
FF = DMAX1(FL,FT)
C basket mechanical seal
EPRE = 0.231614*RE**(0.119679)
Zetat = 6.13296*re**(-0.48622)

```

```

Zeta = 2.0*(8.3483*Zetat+10.06*EPRE)
R54 = (71.79*FF+Zeta)*M4(7)/(64.4*AB**2*144.0*RHO)
C Equivalent resistance coefficient
R5 = 1.0/(1.0/R51+1.0/R53+1.0/R54)
GP(6,8) = 1.0/R5
GP(8,6) = GP(6,8)
C(6,8) = RHO*2.2375/R5
C(8,6) = -C(6,8)
C LINE SEGMENT 8; (Node 7 to Node 8), Flow between inside wall of basket
C and outside of central dip tube
    Ag = 8.424E-3
    Dg = 0.055
    Ab = 0.01533
    Db = 0.086
    E = 0.004
    MDOT = ABS(MDOTI(8))
    PBAR = 0.5*(P(7)+P(8))
    RHO = RHOAR(PBAR,TEMP)
    RE = MDOT*Dg/(Ag*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
        FT = 0.0
    ELSE
        FT = FFAC(E,RE)
    END IF
    Fg = DMAX1(FL,FT)
    RE = MDOT*Db/(Ab*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
        FT = 0.0
    ELSE
        FT = FFAC(E,RE)
    END IF
    FF = DMAX1(FL,FT)
    R = 5.0*((11.85*Fg+1.38)/Ag**2+16.04*FF/Ab**2)*MDOT/(64.4*
1 144.0*RHO)
    GP(7,8) = 1.0/R
    GP(8,7) = GP(7,8)
    C(7,8) = RHO*11.1875/R
    C(8,7) = -C(7,8)
C LINE SEGMENT 9; (Node 2 to Node 7), Flow between outer surface of guide
C cone and basket inner wall
    Af = 4.005E-3
    Df = 0.0104
    E = 0.004
    MDOT = ABS(MDOTI(9))
    PBAR = 0.5*(P(2)+P(7))
    RHO = RHOAR(PBAR,TEMP)
    RE = MDOT*Df/(Af*AMUAR(TEMP))
    FL = 64.0/(RE+0.0001)
    IF(RE .LT. 100.0) THEN
        FT = 0.0
    ELSE
        FT = FFAC(E,RE)

```



```

      END IF
      FF = DMAX1(FL,FT)
      R = (10.0*FF+1.0)*MDOT/(64.4*Af**2*144.0*RHO)
      GP(2,7) = 1.0/R
      GP(7,2) = GP(2,7)
      C(2,7) = 0.0
      C(7,2) = -C(2,7)
C
C   CALCULATE NEW NODAL PRESSURES
C
      CALL SOLVE(NODES,NNM1,GP,C,P,W,G,D)
C
C   SAVE PRESENT FLOW VALUES AND USE NEW NODAL PRESSURES TO CALCULATE
C   NEW FLOWRATES IN THE PIPING SEGMENTS.
      DO 30 I=1,NSEG
        MDOTO(I) = MDOTI(I)
        MDOTI(I) = GP(II(I),JJ(I))*(P(II(I))-P(JJ(I)))-C(II(I),JJ(I))
30    CONTINUE
C
C   EVALUATE CONVERGENCE AND SYSTEM FLOWRATES BY USE OF A WEIGHING
C   FUNCTION WF
C
      ERR = 0.0
      DO 40 I=1,NSEG
        DMDOT(I) = MDOTI(I)-MDOTO(I)
        IF(MDOTI(I) .GT. 0.0) THEN
          ERR = DMAX1(ERR,ABS(DMDOT(I)/MDOTI(I)))
        END IF
        MDOTI(I) = MDOTO(I)+WF*DMDOT(I)
40    CONTINUE
      WRITE(6,*) ICOUNT,ERR
      IF (ICOUNT .LT. 300) THEN
        IF(ICOUNT .LT. 10) GO TO 20
        IF (ERR .GT. EPSN) GO TO 20
      END IF
C   CONVERT MASS FLOW (lb/sec) to SCFM
      DO 50 J=1,NSEG
        SCFM(J) = MDOTI(J)*60.0/RHOr
50    CONTINUE
      DO 60 J=3,7
        M1(J) = M1(J)*60.0/RHOr
        M2(J) = M2(J)*60.0/RHOr
        M3(J) = M3(J)*60.0/RHOr
        M4(J) = M4(J)*60.0/RHOr
C   60    CONTINUE
      DO 70 J=1,N
        PIW(J) = P(J)/0.03613
70    CONTINUE
C
C   PROGRAM OUTPUT
C
      WRITE (8,1)
      WRITE (8,2) ((G(I,J),J=1,N),I=1,N)
      WRITE (8,3)

```

```

C      WRITE (8,4) ((C(I,J),J=1,N),I=1,N)
      WRITE (8,5)
      WRITE (8,6) (I, MDOTI(I), PIW(I), D(I), I=1,N)
      WRITE (8,7) (I, MDOTI(I), I=(N+1),NSEG)
      WRITE(8,8)
      WRITE (8,9) (M1(I), M2(I), M3(I), M4(I), I=3,7)
1      FORMAT (20X, 'ADMITTANCE MATRIX G(i,j)')
2      FORMAT (15F8.3)
3      FORMAT (20X, 'HYDRAULIC HEAD MATRIX C(i,j)')
4      FORMAT (28F4.1)
5      FORMAT (1X, 'NODE', 4X, 'FLOW', 5X, 'PRESSURE', 7X, 'RHS', 9X,
1      'FLS', 9X, 'SCFM', 6X, 'IN-H2O')
6      FORMAT (I5, G12.4, 2G12.6)
7      FORMAT (I5, G12.4)
8      FORMAT (5X, 'Basket flow split')
9      FORMAT (5X, 4G12.6)
      END
      SUBROUTINE SOLVE(NODES,NNM1,GP,C,P,W,G,D)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /SOLV/ NN,NX,NNX,PNX
      DIMENSION
      $ C(NODES,NODES), G(NNM1,NNM1), GP(NODES,NODES), P(NODES),
      $ D(NNM1), PNX(20), NX(20), W(NODES)
C      DETERMINE THE REDUCED (NN X NN) ADMITTANCE MATRIX G(i,j)
C      Remove rows and columns (numbered NX(k)) from G(i,j) for which
C      pressures are specified. L denotes an active row number and
C      M denotes an active column number.
      N = NODES
      MP = 1
      IDR = 0
      DO 80 I=1,NN
35      L = I+IDR
      DO 40 K=1,NNX
      IF(L .EQ. NX(K)) THEN
          IDR = IDR+1
          GO TO 35
      END IF
40      CONTINUE
      IDC = 0
      DO 70 J=1,NN
45      M = J+IDC
      DO 50 KK=1,NNX
      IF(M .EQ. NX(KK)) THEN
          IDC = IDC+1
          GO TO 45
      END IF
50      CONTINUE
C      DIAGONAL ELEMENTS
      IF(L .EQ. M) THEN
          G(I,J) = 0.0
          DO 60 JK=1,N
          G(I,J) = G(I,J)+GP(L,JK)
60      CONTINUE

```

```

C OFF DIAGONAL ELEMENTS
  ELSE
    G(I,J) = -GP(L,M)
  END IF
70 CONTINUE
80 CONTINUE
C
C DETERMINE THE REDUCED RHS (NN X 1) COLUMN MATRIX D(i)
C Add contents of column numbers NX(j) from G(i,j) to RHS.
C L denotes an active row number.
  IDR = 0
  DO 130 I=1,NN
    L = I+IDR
90    D(I) = 0.0
    DO 100 J=1,NNX
      IF(L .EQ. NX(J)) THEN
        IDR = IDR+1
        GO TO 90
      END IF
100    CONTINUE
    DO 110 J=1,NNX
      D(I) = D(I)+GP(L,NX(J))*PNX(J)
110    CONTINUE
    CC = 0.0
    DO 120 K=1,N
      CC = CC+C(L,K)
120    CONTINUE
    D(I) = D(I)+CC+W(L)
130    CONTINUE
C
C SOLVE THE LINEAR EQUATION SET  $G \cdot p = d$  TO OBTAIN NEW PRESSURES P(i)
  CALL GAUSSJ(G,NN,NNM1,D,MP,MP)
C
C UPDATE THE PRESSURE ARRAY INCLUDING THE SPECIFIED PRESSURES
C USED AS BOUNDARY CONDITIONS.
  IDUM = 0
  DO 150 I=1,N
    K = I-IDUM
    P(I) = D(K)
    DO 140 J=1,NNX
      IF(I .EQ. NX(J)) THEN
        P(I) = PNX(J)
        IDUM = IDUM+1
      END IF
140    CONTINUE
150  CONTINUE
  RETURN
  END
  SUBROUTINE GAUSSJ(A,N,NP,B,M,MP)
C Linear equation solution by Gauss-Jordan elimination. A is an input
C matrix of N by N elements, stored in an array of physical dimensions
C NP by NP. B is an input matrix of N by M containing the M right-hand
C side vectors, stored in an physical array of dimensions NP by MP. On
C output, A is replaced by its matrix inverse, and B is replaced by the

```

C corresponding set of solution vectors.

```

C
  IMPLICIT REAL*8(A-H,O-Z)
  PARAMETER (NMAX=50)
  DIMENSION A(NP,NP),B(NP,MP),IPIV(NMAX),INDXR(NMAX),INDXC(NMAX)
C The integer arrays IPIV, INDXR, and INDXC are used for bookkeeping on
C the pivoting. NMAX should be as large as the largest anticipated value
C of N.
  DO 11 J=1,N
    IPIV(J)=0
11  CONTINUE
  DO 22 I=1,N
    BIG=0.
    DO 13 J=1,N
      IF (IPIV(J).NE.1) THEN
        DO 12 K=1,N
          IF (IPIV(K).EQ.0) THEN
            IF (ABS(A(J,K)).GE.BIG) THEN
              BIG=ABS(A(J,K))
              IROW=J
              ICOL=K
            ENDIF
          ELSE IF (IPIV(K).GT.1) THEN
            PAUSE 'Singular matrix'
          ENDIF
        ENDIF
      CONTINUE
    ENDIF
13  CONTINUE
    IPIV(ICOL)=IPIV(ICOL)+1
    IF (IROW.NE.ICOL) THEN
      DO 14 L=1,N
        DUM=A(IROW,L)
        A(IROW,L)=A(ICOL,L)
        A(ICOL,L)=DUM
14  CONTINUE
      DO 15 L=1,M
        DUM=B(IROW,L)
        B(IROW,L)=B(ICOL,L)
        B(ICOL,L)=DUM
15  CONTINUE
    ENDIF
    INDXR(I)=IROW
    INDXC(I)=ICOL
    IF (A(ICOL,ICOL).EQ.0.) PAUSE 'Singular matrix.'
    PIVINV=1./A(ICOL,ICOL)
    A(ICOL,ICOL)=1.
    DO 16 L=1,N
      A(ICOL,L)=A(ICOL,L)*PIVINV
16  CONTINUE
    DO 17 L=1,M
      B(ICOL,L)=B(ICOL,L)*PIVINV
17  CONTINUE
    DO 21 LL=1,N
      IF (LL.NE.ICOL) THEN

```

```

      DUM=A(LL,ICOL)
      A(LL,ICOL)=0.
      DO 18 L=1,N
        A(LL,L)=A(LL,L)-A(ICOL,L)*DUM
18      CONTINUE
      DO 19 L=1,M
        B(LL,L)=B(LL,L)-B(ICOL,L)*DUM
19      CONTINUE
      ENDIF
21      CONTINUE
22      CONTINUE
      DO 24 L=N,1,-1
        IF(INDXR(L).NE.INDXC(L))THEN
          DO 23 K=1,N
            DUM=A(K,INDXR(L))
            A(K,INDXR(L))=A(K,INDXC(L))
            A(K,INDXC(L))=DUM
23          CONTINUE
          ENDIF
24          CONTINUE
      RETURN
      END
      FUNCTION PIPE(XL,D,W,eps,P,T)
C  Function subprogram calculates the linearized loss (Lbf-min/lbm-ft^2) for
C  air flowing in an equivalent length of pipe (XL-ft) of diameter (D-ft)
C  at pressure (P-Lbf/ft^2), temperature (T-deg.R) and flowrate (W-lbm/min).
C  The roughness height is specified by (eps - ft).
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 MDOT
      eD = eps/D
      MDOT = ABS(W)
      RHOR = 0.0763
      RHO = P/(53.35*T)
      XMU = 1.095E-5+(T-460.0)*(1.813E-8-(T-460.0)*(4.375E-12))
      Re = 0.0212*MDOT/(XMU*D)
      IF(Re .GT. 1073.0925) then
        X = -2.0*DLOG10(eD/3.7-5.02/Re*DLOG10(eD/3.7+13.0/Re))
        FF = 1.0/X**2
      ELSE
        FF = 64.0/(Re+0.001)
      END IF
      PIPE = 6.9925E-6*FF*XL*W/(RHO*D**5)
      END

```

APPENDIX C. CC:MAIL, T. D. COOPER TO F. J. HEARD, "HYDROGEN FROM HYDRIDE."

[740] From: Thurman D Cooper at -WHC55 3/31/96 11:46AM (734 bytes: 1 ln)

To: Frederick J Heard at -WHC63

Subject: Hydrogen from Hydride

----- Message Contents -----

Fred,

The correct model for calculating the rate of hydriding and dehydriding is given by Lindner as follows:

$$\alpha = a * \ln(P_o/P) * \exp[-E_a/RT] * (t)$$

where:

α = extent of reaction

$a = 5570$ /min.

$$\log_{10}[P_o] = A/T + B$$

where T is absolute oK and:

	A	B
Hydriding	3473	8.05
Dehydriding	4717	9.46

$E_a = 18.9$ kcal/mole

t = time in minutes

I hope this helps;

Thurman Cooper

DISTRIBUTION SHEET

To	From	Page 1 of 1
Distribution	Process Engineering Analysis	Date 10/7/96
Project Title/Work Order		EDT No. 614692
Spent Nuclear Fuel Project/LB040		ECN No. NA

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
G. D. Bazinet (5)	B4-55	X			
P. J. Bedell	E6-35	X			
P. M. Bourlard	H5-25	X			
F. W. Bradshaw	R3-85	X			
B. S. Carlisle	R3-85	X			
T. D. Cooper	T5-12	X			
R. G. Cowan	R3-86	X			
E. R. Cramer	H0-34	X			
R. L. Deshotels	E6-35	X			
D. R. Duncan (5)	R3-86	X			
S. Edwards	G1-11	X			
J. E. Filip	R3-85	X			
J. R. Frederickson	R3-86	X			
W. M. Funderburke	H5-30	X			
W. D. Gallo	R3-85	X			
L. J. Garvin	R3-85	X			
E. W. Gerber	R3-86	X			
L. H. Goldmann	R3-86	X			
F. J. Heard (7)	H0-34	X			
J. J. Irwin	H0-34	X			
A. T. Kee	R3-86	X			
M. Kummerer	A3-34	X			
B. D. Lorenz	R3-85	X			
M. K. Mahaffey	R3-85	X			
D. W. McNally	G1-11	X			
J. E. Mercado	G1-11	X			
M. G. Mercado	E6-35	X			
C. R. Miska (5)	R3-86	X			
D. M. Ogden	H0-34	X			
R. P. Omberg	H0-40	X			
A. L. Pajunen	R3-86	X			
C. A. Peterson	K9-72	X			
R. S. Popielarczyk	A2-34	X			
J. P. Schmidt	X3-78	X			
P. A. Scott	R3-87	X			
E. J. Shen	R3-86	X			
P. K. Shen	H0-40	X			
J. P. Sloughter	R2-54	X			
D. W. Smith	R3-11	X			
K. E. Smith	R3-85	X			
J. A. Swenson	R3-11	X			
C. A. Thompson	R3-85	X			
M. J. Thurgood	H0-34	X			
J. C. Wiborg	R3-86	X			
W. L. Willis	R3-86	X			
Central Files (Original + 2)	A3-88	X			
PEA File (Burstad 3)	H0-34	X			
SNF Project File	R3-11	X			