The Pennsylvania State University
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DEVELOPMENT OF BURNUP DEPENDENT FUEL ROD MODEL IN COBRA-TF

A Dissertation in
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by
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ABSTRACT

The purpose of this research was to develop a burnup dependent fuel thermal conductivity model within Pennsylvania State University, Reactor Dynamics and Fuel Management Group (RDFMG) version of the subchannel thermal-hydraulics code COBRA-TF (CTF). The model takes into account first, the degradation of fuel thermal conductivity with high burnup; and second, the fuel thermal conductivity dependence on the Gadolinium content for both UO$_2$ and MOX fuel rods. The modified Nuclear Fuel Industries (NFI) model for UO$_2$ fuel rods and Duriez/Modified NFI Model for MOX fuel rods were incorporated into CTF and fuel centerline predictions were compared against Halden experimental test data and FRAPCON-3.4 predictions to validate the burnup dependent fuel thermal conductivity model in CTF. Experimental test cases from Halden reactor fuel rods for UO$_2$ fuel rods at Beginning of Life (BOL), through lifetime without Gd$_2$O$_3$ and through lifetime with Gd$_2$O$_3$ and a MOX fuel rod were simulated with CTF. Since test fuel rod and FRAPCON-3.4 results were based on single rod measurements, CTF was run for a single fuel rod surrounded with a single channel configuration. Input decks for CTF were developed for one fuel rod located at the center of a subchannel (rod-centered subchannel approach). Fuel centerline temperatures predicted by CTF were compared against the measurements from Halden experimental test data and the predictions from FRAPCON-3.4.

After implementing the new fuel thermal conductivity model in CTF and validating the model with experimental data, CTF model was applied to steady state and transient calculations. 4x4 PWR fuel bundle configuration from Purdue MOX benchmark was used to apply the new model for steady state and transient calculations. First, one of each high burnup UO$_2$ and MOX fuel rods from 4x4 matrix were selected to carry out single fuel rod calculations and fuel centerline temperatures predicted by CTF/TORT-TD were compared against CTF /TORT-TD
FRAPTRAN predictions. After confirming that the new fuel thermal conductivity model in CTF worked and provided consistent results with FRAPTRAN predictions for a single fuel rod configuration, the same type of analysis was carried out for a bigger system which is the 4x4 PWR bundle consisting of 15 fuel pins and one control guide tube. Steady-state calculations at Hot Full Power (HFP) conditions for control guide tube out (unrodded) were performed using the 4x4 PWR array with CTF/TORT-TD coupled code system. Fuel centerline, surface and average temperatures predicted by CTF/TORT-TD with and without the new fuel thermal conductivity model were compared against CTF/TORT-TD/FRAPTRAN predictions to demonstrate the improvement in fuel centerline predictions when new model was used. In addition to that constant and CTF dynamic gap conductance model were used with the new thermal conductivity model to show the performance of the CTF dynamic gap conductance model and its impact on fuel centerline and surface temperatures.

Finally, a Rod Ejection Accident (REA) scenario using the same 4x4 PWR array was run both at Hot Zero Power (HZP) and Hot Full Power (HFP) condition, starting at a position where half of the control rod is inserted. This scenario was run using CTF/TORT-TD coupled code system with and without the new fuel thermal conductivity model. The purpose of this transient analysis was to show the impact of thermal conductivity degradation (TCD) on feedback effects, specifically Doppler Reactivity Coefficient (DRC) and, eventually, total core reactivity.
# TABLE OF CONTENTS

LIST OF FIGURES ............................................................................................................................... xi

LIST OF TABLES ................................................................................................................................ xix

ACKNOWLEDGMENTS ..................................................................................................................... xxi

CHAPTER 1 INTRODUCTION ........................................................................................................... 1
  1.1 Background ............................................................................................................................. 1
  1.2 Statement of Objective ............................................................................................................ 3
  1.3 Dissertation Outline ................................................................................................................ 5
  1.4 References ............................................................................................................................... 7

CHAPTER 2 LITERATURE REVIEW ............................................................................................... 9
  2.1 Introduction ............................................................................................................................. 9
  2.2 Fuel Thermal Conductivity Model Comparisons and Literature Review ......................... 9
  2.3 COBRA-TF (CTF) Background and History ................................................................. 19
  2.4 FRAPCON-3.4 Steady State Fuel Performance Code ...................................................... 20
  2.5 Physical Mechanisms Occurring in The Fuel Rod During High Burnup ..................... 24
    2.5.1 Cladding Degradation Mechanisms During High Burnup ........................................ 24
    2.5.2 Fuel Pellet Degradation Mechanisms During High Burnup .................................... 27
  2.6 Mechanisms of Thermal Conductivity Degradation During High Burnup ................. 28
  2.7 References ............................................................................................................................... 30

CHAPTER 3 SENSITIVITY ANALYSIS OF BWR FUEL ROD THERMAL PROFILE .............. 36
  3.1 Introduction ............................................................................................................................. 36
  3.2 Analytical Solution to Cylindrical Fuel Rod Radial Temperature Profile ...................... 37
8.4 References ........................................................................................................................................... 192

CHAPTER 9 .................................................................................................................................................. 193

CONCLUSIONS AND FUTURE WORK ........................................................................................................ 193

9.1 Conclusions ........................................................................................................................................ 193
9.2 Summary of Contributions ................................................................................................................ 198
9.3 Suggestions for Future Work ............................................................................................................ 199

APPENDIX A ............................................................................................................................................... 200

GADOLINIUM OXIDE LATTICE STRUCTURE ............................................................................................. 200

A.1 References ......................................................................................................................................... 202

APPENDIX B ............................................................................................................................................... 203

CTF, FRAPTRAN and TORT-TD THREE CODES COUPLING SYSTEM ................................................... 203

B.1 References ......................................................................................................................................... 205

APPENDIX C ............................................................................................................................................... 206

CTF NUCLEAR FUEL ROD DEFORMATION MODEL ................................................................................. 206

C.1 Fuel Pellet Cracking and Sintering Effect on Conductivity ................................................................. 206
C.2 Fuel Pellet and Cladding Expansion Effects on Gap Thickness ......................................................... 207
C.3 Fuel and Clad Thermal Expansion .................................................................................................... 207
C.4 Fuel Pellet Relocation ....................................................................................................................... 208
C.5 Cladding Elastic Deformation ........................................................................................................ 208
C.6 References ......................................................................................................................................... 209
APPENDIX D

CTF PELLET-CLADDING DYNAMIC GAP CONDUCTANCE MODEL

D.1 CTF Pellet-Cladding Gap Conductance Model
D.1.1 Radiant Heat Transfer
D.1.2 Conduction Heat Transfer in the Fill Gas
D.1.3 Pellet-Cladding Contact Conductance
D.2 Impact of Gap Conductance on Fuel Temperature Profile
D.3 Dynamic Gap Conductance Calculation
D.4 Uniform Gap Conductance Calculation
D.5 Comparison and Conclusions
D.6 References

APPENDIX E

IMPACT OF RADIAL NODAL/AVERAGE THERMAL CONDUCTIVITY ON FUEL TEMPERATURE PROFILE

E.1 References

APPENDIX F

CTF SINGLE CHANNEL SAMPLE INPUT DECK

APPENDIX G

CODE UNCERTAINTIES

G.1 Fuel Performance Code Uncertainties
G.1.2 Output Uncertainties
G.2 Bundle Thermal Hydraulics Code Uncertainties ................................................................. 236
  G.2.1 Input Uncertainties ..................................................................................................... 236
  G.2.2 Output Uncertainties ............................................................................................... 237
G.3 References ..................................................................................................................... 237
LIST OF FIGURES

Figure 3-1 Thermal resistance demonstration for a cylindrical fuel pin ......................................38

Figure 3-2 Radial Fuel Temperature Profile for a BWR Rod using Different Fuel
Thermal Conductivity Values at q' = 16.4 kW/m .................................................................42

Figure 3-3 Radial Fuel Temperature Profile for a BWR Rod using Different Fuel
Thermal Conductivity Values at q' = 32.8 kW/m .................................................................42

Figure 3-4 Radial Fuel Temperature Profile for a BWR Rod using Different Fuel
Thermal Conductivity Values at q' = 49.2 kW/m .................................................................43

Figure 3-5 Radial Fuel Temperature Deviation Profile from the BWR Reference Test
Case at q' = 16.4 kW/m ........................................................................................................43

Figure 3-6 Radial Fuel Temperature Deviation Profile from the BWR Reference Test
Case at q' = 32.8 kW/m ........................................................................................................44

Figure 3-7 Radial Fuel Temperature Deviation Profile from the BWR Reference Test
Case at q' = 49.2 kW/m ........................................................................................................44

Figure 3-8 Fuel Centerline Temperature vs. Fuel Thermal Conductivity at the Three
Power Levels ..........................................................................................................................45

Figure 3-9 Radial Temperature Profile for a BWR Rod with Changing the Gap
Conductance at q' = 16.4 kW/m .........................................................................................48

Figure 3-10 Radial Temperature Profile for a BWR Rod with Changing the Gap
Conductance at q' = 32.8 kW/m .........................................................................................48

Figure 3-11 Radial Temperature Profile for a BWR Rod with Changing the Gap
Conductance at q' = 49.2 kW/m .........................................................................................49

Figure 3-12 Radial Temperature Deviation Profile from the BWR Reference Test Case
by Changing Gap Conductance at q' = 16.4 kW/m ..........................................................49

Figure 3-13 Radial Temperature Deviation Profile from the BWR Reference Test Case
by Changing Gap Conductance at q' = 32.8 kW/m ..........................................................50

Figure 3-14 Radial Temperature Deviation Profile from the BWR Reference Test Case
by Changing Gap Conductance at q' = 49.2 kW/m ..........................................................50

Figure 3-15 Fuel Centerline Temperature vs. Gap Conductance at q' = 16.4 kW/m, 33.8
kW/m, and 49.2 kW/m .......................................................................................................51

Figure 3-16 Radial Fuel Temperature Profile for a BWR Rod with Changing the Fuel
Pellet Radius at q' = 16.4 kW/m .........................................................................................53
Figure 3-17 Radial Temperature Profile for a BWR Rod with Changing the Fuel Pellet Radius at $q' = 32.8$ kW/m .................................................................................................................. 54

Figure 3-18 Radial Temperature Profile for a BWR Rod with Changing the Fuel Pellet Radius at $q' = 49.2$ kW/m .................................................................................................................. 54

Figure 3-19 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Fuel Pellet Radius at $q' = 16.4$ kW/m ................................................................. 55

Figure 3-20 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Fuel Pellet Radius at $q' = 32.8$ kW/m ................................................................. 55

Figure 3-21 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Fuel Pellet Radius at $q' = 49.2$ kW/m ................................................................. 56

Figure 3-22 Fuel Centerline Temperature vs. Fuel Pellet Radius at $q' = 16.4$, $32.8$, and $49.2$ kW/m .......................................................................................................................... 56

Figure 3-23 Radial Temperature Profile for a BWR Rod with Changing Clad Inside Radius at $q' = 16.4$ kW/m ................................................................................................................. 59

Figure 3-24 Radial Temperature Profile for a BWR Rod with Changing Clad Inside Radius at $q' = 32.8$ kW/m ................................................................................................................. 59

Figure 3-25 Radial Temperature Profile for a BWR Rod with Changing Clad Inside Radius at $q' = 49.2$ kW/m ................................................................................................................. 60

Figure 3-26 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Clad Inside Radius at $q' = 16.4$ kW/m ................................................................. 60

Figure 3-27 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Clad Inside Radius at $q' = 32.8$ kW/m ................................................................. 61

Figure 3-28 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Clad Inside Radius at $q' = 49.2$ kW/m ................................................................. 61

Figure 3-29 Fuel Centerline Temperature vs. Clad Inside Radius at $q' = 16.4$, $32.8$, and $49.2$ kW/m .......................................................................................................................... 62

Figure 4-2 MATPRO-11 and Modified NFI Thermal Conductivity Models for UO$_2$ as a Function of Temperature, [4] ........................................................................................................ 74

Figure 4-3 MATPRO-11 Model to Data Comparison for Thermal Conductivity of Unirradiated UO$_2$ [4] .......................................................................................................... 75

Figure 4-4 Modified NFI Model to Data Comparison for Thermal Conductivity of Unirradiated UO$_2$ [4] .......................................................................................................... 75

Figure 4-5 MATPRO-11 Model to Data Comparison for Thermal Conductivity of Irradiated UO$_2$ [4] .......................................................................................................... 76
Figure 4-6 MATPRO-11 and Duriez/Modified NFI Thermal Conductivity Models for MOX as a Function of Temperature. [4] ........................................................................................................ 78

Figure 4-7 MATPRO-11 Model to Data Comparison for Thermal Conductivity of MOX Fuel [4] .................................................................................................................. 79

Figure 4-8 Duriez/Modified NFI Model to Data Comparison for Thermal Conductivity of MOX Fuel [4] ........................................................................................................ 80

Figure 4-9 Comparison of Fuel Thermal Conductivities between CTF and MATPRO-11 .... 83

Figure 4-10 Comparison of Fuel Thermal Conductivity Models between CTF, MATPRO-11, and the Modified NFI .................................................................................. 83

Figure 4-11 Comparison of Fuel Thermal Conductivity Models between CTF, MATPRO-11, and the Duriez/Modified NFI ........................................................................... 84

Figure 4-12 Modified NFI Model Thermal Conductivity as a Function of Temperature with Increasing Gadolinium Concentration (at 0 GWd/MTU) .............................. 86

Figure 4-13 Modified NFI Model Thermal Conductivity as a Function of Temperature with Increasing Gadolinium Concentration (at 30 GWd/MTU) .............................. 87

Figure 4-14 Modified NFI Model Thermal Conductivity as a Function of Temperature with Increasing Gadolinium Concentration (at 60 GWd/MTU) .............................. 88

Figure 4-15 Effect of Exposure on Fuel Thermal Conductivity as a Function of Temperature ......................................................................................................................... 89

Figure 4-16 Effect of Exposure on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model .................................................. 91

Figure 4-17 Effect of Gadolinium Concentration on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model (at 0 GWd/MTU) .................................................................................................................. 91

Figure 4-18 Effect of Gadolinium Concentration on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model (at 30 GWd/MTU) .................................................................................................................. 92

Figure 4-19 Effect of Gadolinium Concentration on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model (at 60 GWd/MTU) .................................................................................................................. 92

Figure 5-1 Comparisons of Steady-State Fuel Thermal Conductivities vs. Fuel Temperature for Single center PWR at 0 GWd/MTU and 0 w/o Gd ........................................... 97

Figure 5-2 Comparisons of CTF predicted Fuel Thermal Conductivities vs. Fuel Temperature for Single Center PWR at Different Gd Concentration and Exposure Levels .......................................................... 98
**Figure 5-3** Comparisons of CTF predicted Fuel Thermal Conductivities vs. Fuel Temperature for Single Center PWR at Different Gd Concentration and 0 GWd/MTU ................................................................. 99

**Figure 5-4** Comparisons of CTF predicted Fuel Thermal Conductivities to FRAPCON-3.4 Predictions for PWR Rod at Different Gd Concentration and 30 GWd/MTU ............ 99

**Figure 6-1** IFA-432r1 BOL UO₂ Fuel Centerline Temperature Predictions .................. 103

**Figure 6-2** IFA-432r1 UO₂ LHGR vs. Fuel Rod Average Burnup ................................. 104

**Figure 6-3** Fuel Centerline Temperature vs. Rod Average Burnup for IFA-432r1 ........ 105

**Figure 6-4** Predicted vs. Measured Fuel Centerline Temperature for IFA-432r1 UO₂ at 45 GWd/MTU ................................................................................................................. 105

**Figure 6-5** Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-432r1 UO₂ at 45 GWd/MTU ................................. 106

**Figure 6-6** Linear Heat generation Rate vs. Rod Average Burnup for IFA-681r2 UO₂+2%Gd₂O₃ .................................................. 108

**Figure 6-7** Fuel Centerline Temperatures vs. Rod Average Burnup for IFA-681r2 UO₂+2%Gd₂O₃ .................................................. 108

**Figure 6-8** Predicted vs. Measured Fuel Centerline Temperature for IFA-681r2 UO₂+2%Gd₂O₃ .................................................. 109

**Figure 6-9** Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-681r2 ............................................................. 109

**Figure 6-10** Linear Heat generation Rate vs. Rod Average Burnup for IFA-681r3 UO₂+8%Gd₂O₃ .................................................. 111

**Figure 6-11** Fuel Centerline Temperatures vs. Rod Average Burnup for IFA-681r3 UO₂+8%Gd₂O₃ .................................................. 112

**Figure 6-12** Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-681r3 ............................................................. 112

**Figure 6-13** Predicted vs. Measured Fuel Centerline Temperature for IFA-681r3 UO₂+8%Gd₂O₃ .................................................. 113

**Figure 6-14** Linear Heat generation Rate vs. Rod Average Burnup for IFA-610r2 MOX Fuel Rod ................................................ 114

**Figure 6-15** Fuel Centerline Temperatures vs. Rod Average Burnup for IFA-610r2 MOX Fuel Rod ................................................ 115
Figure 6-16 Predicted vs. Measured Fuel Centerline Temperature for IFA-610r2 MOX Fuel Rod

Figure 6-17 Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-610r2

Figure 6-18 Predicted vs. Measured Fuel Centerline Temperature for IFA-432r1 BOL, IFA-432r1 burnup, IFA-681r2 UO₂+2%Gd₂O₃, 681r3 UO₂+8%Gd₂O₃ and IFA-610r2 MOX

Figure 6-19 Normalized Fuel Centerline Temperature vs. Rod Average Burnup for IFA-432r1 BOL, IFA-432r1 burnup, IFA-681r2 UO₂+2%Gd₂O₃, IFA-681r3 UO₂+8%Gd₂O₃ and IFA-610r2 MOX

Figure 6-20 Descriptive Statistics for CTF with IFRAP=0 Normalized Fuel Centerline Temperature

Figure 6-21 Descriptive Statistics for CTF with IFRAP=1 Normalized Fuel Centerline Temperature

Figure 6-22 Descriptive Statistics for FRAPCON-3.4 Normalized Fuel Centerline Temperature

Figure 7-1 Single fuel rod centered in a single channel

Figure 7-2 Fuel Centerline Temperature vs. Axial Position for UO₂ High Burnup Fuel Rod

Figure 7-3 CTF vs. FRAPTRAN Fuel Centerline Temperature

Figure 7-4 Fuel Pellet Surface Temperature vs. Axial Position for UO₂ High Burnup Fuel Rod

Figure 7-5 Gap Conductance vs. Axial Position for UO₂ High Burnup Fuel Rod

Figure 7-6 Relative Power vs. Normalized Fuel Pellet Radius

Figure 7-7 Axial Power Profile

Figure 7-8 Fuel Centerline Temperature vs. Axial Position for MOX High Burnup Fuel Rod

Figure 7-9 CTF vs. FRAPTRAN Fuel Centerline Temperature

Figure 7-11 Gap Conductance vs. Axial Position for MOX High Burnup Fuel Rod

Figure 7-12 Radial Power Profile vs. Normalized Fuel Pellet Radius

Figure 7-13 4x4 PWR Pin Array and Subchannel Configuration [2]
Figure 7-14 TORT-TD Assembly Arrangement [2] ............................................................... 141

Figure 7-15 Control Rod Insertion during Rod Ejection Accident [2] ............................ 142

Figure 7-16 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6 (Low burnup MOX) .............................................................................................. 146

Figure 7-17 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6 (Low burnup MOX) .............................................................................................. 147

Figure 7-18 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 7 (High burnup MOX) .............................................................................................. 148

Figure 7-19 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 7 (High burnup MOX) .............................................................................................. 149

Figure 7-20 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10 (Low burnup UO2) ............................................................................................... 152

Figure 7-21 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10 (Low burnup UO2) ............................................................................................... 153

Figure 7-22 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11 (High burnup UO2) ............................................................................................... 154

Figure 7-23 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11 (High burnup UO2) ............................................................................................... 155

Figure 7-24 CTF vs. FRAPTRAN Fuel Temperature Comparisons for All Rods ............... 156

Figure 7-25 CTF vs. FRAPTRAN RPD for All Rods ............................................................ 157

Figure 7-26 CTF vs. FRAPTRAN RPD for All Rods ............................................................ 158

Figure 7-27 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6 .............................................................................................................................. 160

Figure 7-28 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6 .............................................................................................................................. 161

Figure 7-29 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 7 .............................................................................................................................. 162

Figure 7-30 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 7 .............................................................................................................................. 163

Figure 7-31 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10 .............................................................................................................................. 164
Figure 7-32 CTF with IFRAP= 1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10 .............................................................................................................................. 165

Figure 7-33 CTF with IFRAP= 0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11 .............................................................................................................................. 166

Figure 7-34 CTF with IFRAP= 1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11 .............................................................................................................................. 167

Figure 7-35 CTF vs. FRAPTRAN Fuel Temperature Comparisons for All Rods .......... 168

Figure 8-1 REA Transient Results at HZP condition, CTF uses uniform RPD and constant hgap .................................................................................................................... 178

Figure 8-2 REA Transient Results at HZP condition, CTF uses uniform RPD and dynamic hgap ................................................................................................................... 179

Figure 8-3 REA Transient Results at HZP condition, CTF uses FRAPTRAN RPD and constant hgap .................................................................................................................... 180

Figure 8-4 REA Transient Results at HZP condition, CTF uses FRAPTRAN RPD and dynamic hgap ................................................................................................................... 181

Figure 8-5 REA Transient Total Power Results at HFP condition ........................................ 185

Figure 8-6 REA Transient Fuel Average Temperature Results at HFP condition .............. 186

Figure 8-7 REA Peak Fuel Enthalpy .................................................................................... 186

Figure 8-8 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 7 (IFRAP=0) .................................................................................................................. 187

Figure 8-9 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 7 (IFRAP=1) .................................................................................................................. 187

Figure 8-10 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 11 (IFRAP=0) .................................................................................................................. 188

Figure 8-11 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 11(IFRAP=1) .................................................................................................................. 188

Figure 8-12 REA Transient Fuel Centerline Temperature Differences at HFP condition for Rod 7 .......................................................................................................................... 189

Figure 8-13 Delta ta Fuel Centerline Temperature for Rod 7 during HFP REA using CTF with IFRAP=0 .................................................................................................................. 189

Figure 8-14 Delta ta Fuel Centerline Temperature for Rod 7 during HFP REA using CTF with IFRAP=1 .................................................................................................................. 190
Figure A-1 Demonstration of Gadolinium Oxide Crystal Structures and Phases .......................... 201
Figure A-2 Sample Demonstration of Cubic Lattice Configurations ........................................ 201
Figure B-1 Coupling Interface Structure [1] ................................................................................ 204
Figure B-2 Data Transfer between CTF and FRAPCON with TORT-TD Feedback ..................... 205
Figure C-1 A Sample of Cracked Uranium Oxide Fuel [2] ............................................................. 207
Figure D-1 Components of the Pellet-Cladding Gap Conductance for IFA-681-r2 rod .............. 211
Figure D.2 Demonstration of the Temperature Jump on Fuel Pellet and Clad Surfaces [1] ... 213
Figure D-3 Radial Power Profile vs. Radial Node for IFA-681-r2 UO_2/Gd_2O_3 ..................... 216
Figure D-4 Gap Conductance Profiles CTF Dynamic Gap vs. FRAPCON-3.4 for IFA-681-r2 UO_2/Gd_2O_3 .......................................................... 216
Figure D-5 Radial Temperature Profile Comparison for CTF Dynamic Gap vs. FRAPCON .......... 217
Figure D-6 Radial Thermal Conductivity Profile Comparison for CTF Dynamic Gap vs. FRAPCON .......................................................... 218
Figure D-7 Radial Temperature Profile Comparison for CTF Constant Gap vs. FRAPCON .......... 219
Figure D-8 Radial Thermal Conductivity Profile Comparison for CTF Constant Gap vs. FRAPCON .......................................................... 219
Figure D-9 Radial Temperature Profiles Comparison for CTF Dynamic and Constant Gap vs. FRAPCON .......................................................... 221
Figure E-1 Radial Fuel Nodes and Rings for a Single Fuel Rod Temperature Profile Calculations .................................................................................. 223
Figure E-2 Comparison of Radial Nodal vs. Radial Average Thermal Conductivities ............ 225
Figure E-3 Comparison of Radial Temperature Profiles for Nodal vs. Average Thermal Conductivities .................................................................................. 225
LIST OF TABLES

Table 2-1 Summary of Thermal Conductivity Equations............................................................22
Table 3-1 Reference Test Case Values Used at Each Power Level.................................39
Table 3-2 Operating Domain for Each Parameter used in the Sensitivity Analysis Test Matrix...............................................................................................................................39
Table 3-4 Test Points used at Each Power Level.................................................................41
Table 3-5 Maximum Radial Temperature Deviation at Each Power Level..................41
Table 3-6 Test Points used at Each Power level.................................................................46
Table 3-7 Percent (%) Temperature Drop (delta T) from the Reference Case at Each Power Level.....................................................................................................................47
Table 3-8 Temperature Drop (deltaT) from the Reference Case at Each Power Level for Different Gap Conductance Values .................................................................................47
Table 3-9 Fuel Centerline Temperature at Different Power Levels..............................47
Table 3-10 Maximum Fuel Centerline Temperature at Each Power Level ....................52
Table 3-11 Test Points used at Each Power Level...............................................................53
Table 3-12 Percent (%) Change in Temperature from the Reference Case at Each Power Level................................................................................................................................57
Table 3-13 Test Points used at Each Power Level...............................................................58
Table 3-14 Fuel Rod Temperature Profile vs. Fuel Parameters Relationship-Impact Matrix...............................................................................................................................64
Table 6-1 Statistical Summary of P/M Ratios for All Calculations....................................119
Table 7-1 As-manufactured cold fuel dimensions [2] .........................................................135
Table 7-2 Input parameters for both of the fuel types [2] ...................................................136
Table 7-3 Nodalization of FRAPCON models for both of the fuel types [2] ....................136
Table 7-4 Fuel parameters for each fuel type [2]...............................................................136
Table 7-5 FRAPTRAN input parameters for all rods [2] ..................................................137
Table 7-6 FRAPCON initialization time for each fuel rod type [2] ....................................137
Table 7-7 Nodalization inputs for FRAPTRAN [2] ................................................................. 137
Table 7-8 Sub-channel geometry type information [2] .......................................................... 138
Table 7-9 Sub-channel horizontal connection type information [2] ........................................ 138
Table 7-10 Modeling options used in CTF [2] ........................................................................ 138
Table 7-11 CTF boundary conditions [2] ............................................................................... 138
Table 7-12 CTF radial and axial nodalization [2] .................................................................... 139
Table 7-13 CTF spacer grid information [2] .......................................................................... 139
Table 7-14 CTF fuel rod models ............................................................................................ 139
Table 7-15 CTF fuel properties [2] ....................................................................................... 140
Table 7-16 TORT-TD model properties [2] ......................................................................... 140
Table 7-17 TORT-TD axial nodalization [2] ........................................................................... 140
Table 7-18 Cross-section libraries [2] .................................................................................. 142
Table 7-19 Initial steady-state power [2] .............................................................................. 142
Table 7-20 Multiplication factor results ................................................................................ 171
Table 7-21 Statistics for CTF with IFRAP=0 results ............................................................... 171
Table 8-1 HZP REA output parameters for the three models .................................................. 175
Table 8-2 Alternate Calculation Summary for Doppler Reactivity Coefficient .................... 183
Table 8-3 HFP output parameters for the two CTF models .................................................... 185
Table A-1 Gadolinium Oxide physical and structural properties ........................................... 201
Table G-1 Core Boundary Condition Variations .................................................................... 235
Table G-2 Core Boundary Condition Variations .................................................................... 236
Table G-3 Geometry Variations ............................................................................................ 236
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CHAPTER 1

INTRODUCTION

1.1 Background

During last decade there has been a trend going towards longer fuel cycles, transition from 18 to 24 months, extended power uprates (EPU) and increasing complexity in commercial fuel designs to improve fuel efficiency. All these changes resulted in higher burnup fuel operations which caused some fuel performance issues and industry challenges such as development of a porous pellet rim and decreased thermal conductivity with increased burnup. In addition to that, the extension to the higher exposure increased the impact of exposure dependent effects such as the increase in rod internal pressure due to fission gas release and increased hydrogen uptake due to increased corrosion of the cladding. Moreover, additional experimental databases for Light Water Reactor (LWR) fuel brought new experimental observations at fuel peak nodal burnups above 40 GWd/MTU. All these changes indicated the need for revised design criteria and possible changes to licensing requirements for normal operation, including anticipated operational occurrences, and accidents such as Loss of Coolant Accident (LOCA) and Reactivity Insertion Accident (RIA). Interest in these issues is prompted by the results of RIA experiments and concerns raised by U.S. Nuclear Regulatory Commission (NRC) for high burnup operation [1, 2, 3, 4, 5, 6, 7].

The ability to accurately calculate the performance of LWR fuel rods under long-term burnup conditions is a major objective of the reactor safety research program conducted by the U.S. NRC [8, 9, 10, 11]. To achieve this goal, the U.S. NRC has sponsored an extensive program of code development and benchmarking studies with the experimental data to validate code performances. The computer code developed to calculate the long-term burnup response of a single rod under steady state operation is FRAPCON [8, 9]. The computer code developed to
calculate the response of a single rod to operational transients and hypothetical accidents is FRAPTRAN [10, 11]. The ongoing development of these two codes has been performed by U.S. NRC under contract with Pacific Northwest National Laboratory (PNNL). The NRC uses these codes primarily in their review of fuel performance codes and fuel design changes that are submitted for licensing analyses by fuel vendors.

The model for degradation of fuel thermal conductivity with high burnup already exists in 1D fuel performance codes FRAPCON and FRAPTRAN. Whereas, subchannel thermal hydraulics codes such as COBRA-TF (COolant Boiling in Rod Arrays-Two Fluid) still uses the old UO₂ material properties from 1979, which do not include the burnup effects on thermal conductivity. Inclusion of the high burnup degradation of thermal conductivity is important since it will affect the fuel centerline temperature predictions and thus changes in the steady state and transient operation margins. The thermal conductivity degradation in high burnup fuel delays the radial heat transfer, and leads to an undesired increase in fuel temperature under steady state reactor operations [4]. In addition to that, tests performed in the Nuclear Safety Research Reactor (NSRR) in Japan showed that occurrence of boiling crises at the clad-to-coolant interface are affected by the changes in the heat transfer properties of the fuel rod [4]. A boiling crisis, or burnout, is a transition from efficient clad-to-coolant heat transfer to a regime with film boiling and impaired heat transfer at a certain critical heat flux [4]. The transition is termed departure from nucleate boiling (DNB) when the coolant is a single phase liquid or subcooled boiling in pressurized water reactors (PWRs), and dryout when the coolant comprises both liquid and steam in boiling water reactors (BWRs). It has been found that boiling crises are suppressed or delayed, when radial heat transfer is delayed by a large pellet-clad gap or a thick layer of oxide at the cladding surface [4]. Degradation of fuel thermal conductivity will delay the heat transfer from fuel to cladding outside surface and will have a similar effect on the occurrence of boiling crises;
also due to the insufficient radial heat conduction through the pellet it might also cause fuel melting.

1.2 Statement of Objective

The purpose of this research is to develop a burnup dependent fuel thermal conductivity model within the Pennsylvania State University Reactor Dynamics and Fuel Management Group (PSU/RDFMG) version of the subchannel thermal-hydraulics code COBRA-TF (CTF). The model will take into account first, the degradation of fuel thermal conductivity with high burnup; and second, the fuel thermal conductivity dependence on the Gadolinium content for both UO₂ and mixed oxide fuel (MOX) rods. The modified Nuclear Fuel Industries (NFI) model for UO₂ fuel rods [8] and Duriez/Modified NFI Model for MOX fuel rods [8] be incorporated into CTF and fuel centerline predictions will be compared against Halden experimental test data [9] and FRAPCON-3.4 [9] predictions to validate the burnup dependent fuel thermal conductivity model in CTF. Experimental test cases from Halden reactor fuel rods [9] for UO₂ fuel rods at Beginning of Life (BOL), through lifetime without Gd₂O₃ and through lifetime with Gd₂O₃ and a MOX fuel rod will be simulated with CTF. Since test fuel rod and FRAPCON-3.4 results are based on a single rod measurements, CTF will be run for a single fuel rod surrounded with a single channel coolant configuration. Input decks for CTF will be developed for one fuel rod located at the center of a subchannel (rod-centered subchannel approach). Fuel centerline temperatures predicted by CTF will be compared against the measurements from Halden experimental test data and the predictions from FRAPCON-3.4.

After implementing the new fuel thermal conductivity model in CTF and validating the model with experimental data, CTF model will be applied to steady state and transient calculations. 4x4 PWR fuel bundle configuration from Purdue MOX benchmark [13] will be used to apply the new model for steady state and transient calculations. First one of the high burnup
UO₂ and MOX fuel rods from 4x4 matrix will be selected to carry out single fuel rod calculations and fuel centerline temperatures predicted by CTF/TORT-TD [14] coupled code system will be compared against predictions of the CTF/TORT-TD/FRAPTRAN [14] coupled code system. In the first calculations, fuel temperature distribution will be obtained using the simplified nuclear fuel rod model of CTF; whereas in the second calculations the fuel performance code FRAPTRAN will be used. After confirming that the new fuel thermal conductivity model in CTF works and gives consistent results with FRAPTRAN predictions for a single fuel rod configuration, the same type of analysis will be carried out for a bigger system which is the 4x4 PWR bundle consisting of 15 fuel pins and one control guide tube. Steady–state calculations at Hot Full Power (HFP) conditions for control guide tube out (unrodded) will be run using the 4x4 PWR array with CTF/TORT-TD coupled code system. Fuel centerline, surface and average temperatures predicted by CTF/TORT-TD with and without the new fuel thermal conductivity model will be compared against CTF/TORT-TD/FRAPTRAN predictions to demonstrate the improvement in fuel centerline predictions when new model is used. In addition to that constant and CTF dynamic gap conductance model will be used with the new thermal conductivity model to show the performance of the CTF dynamic gap conductance model and its impact on fuel centerline and surface temperatures.

Finally, a Rod Ejection Accident (REA) scenario using the same 4x4 PWR array will be run both at Hot Zero Power (HZP) and Hot Full Power (HFP) condition, starting at half of the control rod is inserted position. This scenario will be run using CTF/TORT-TD coupled code system with and without the new fuel thermal conductivity model. The purpose of this transient analysis is to show the impact of thermal conductivity degradation (TCD) on feedback effects, specifically Doppler Reactivity Coefficient (DRC) and eventually total core reactivity.
1.3 Dissertation Outline

The organization of the dissertation will be as follows:

Chapter 1 states the background of the research topic and statement of objective of the dissertation. It briefly explains the importance of the research.

Chapter 2 gives an overall summary of the literature review conducted for this research study. It explains the previous studies conducted in the same area.

Chapter 3 presents the sensitivity study that has been performed on the fuel rod parameters affecting the fuel radial temperature profile.

Chapter 4 describes and compares the fuel thermal conductivity models of CTF and FRAPCON-3.4. It also shows the thermal conductivity database created for the modified NFI model in FRAPCON-3.4 to demonstrate the thermal conductivity versus temperature domain at different exposure and gadolinium concentration levels. CTF predicted thermal conductivities are compared against the prediction from FRAPCON-3.4 modified NFI model in the same temperature domain.

Chapter 5 shows the benchmark studies performed on fuel thermal conductivity between the updated CTF with modified NFI model and FRAPCON-3.4. A PWR example test case is selected from FRAPTRAN Integral Assessment [11] and fuel thermal conductivities predicted from FRAPCON-3.4 and CTF are compared. It is confirmed that modified NFI model in CTF is implemented properly.

Chapter 6 summarizes the results for the CTF new burnup dependent fuel thermal conductivity model implementation and validation against the Halden experimental test data. Five fuel rods are selected from FRAPCON Integral Assessment [9] to compare the fuel centerline temperatures from CTF against Halden experimental test data and FRAPCON predictions: (1)
During first ramp to power (BOL, UO$_2$), (2) throughout life (burnup, UO$_2$), (3) Burnup with 2% Gd$_2$O$_3$, (4) Burnup with 8% Gd$_2$O$_3$ and (5) MOX case with burnup. These five rods are selected because they are representatives for all different conditions including BOL and burnup conditions as well as different Gd concentrations and different fuel rods, UO$_2$ and MOX rods. In addition to that the rods selected for comparison are solid rods so that a good comparison can be made for the fuel centerline temperatures.

Chapter 7 summarizes the single and multi-channel steady state calculations performed by using CTF/TORT-TD with and without the new fuel burnup dependent thermal conductivity model. Fuel centerline, surface and average temperature results predicted by CTF/TORT-TD are compared against CTF/TORT-TD/FRAPTRAN predictions.

Chapter 8 demonstrates the rod ejection accident (REA) analysis run for 4x4 PWR pin array both at Hot Zero Power (HZP) and Hot Full Power (HFP) condition, starting at half of the control rod is inserted position.

Chapter 9 summarizes conclusions, observations and future work for all the analysis performed throughout the dissertation.
1.4 References


CHAPTER 2
LITERATURE REVIEW

2.1 Introduction

Chapter 2 discusses the literature review that was performed to summarize the historical studies related to the research topic presented in this dissertation. A detailed literature review was performed to investigate what was done in the past and what were the conclusions and recommendations from the previous studies and how they can help to establish the direction of this research. CTF and FRAPCON-3.4 thermal conductivity models were also explained briefly in this chapter. The detailed model descriptions for both CTF and FRAPCON-3.4 will be provided in Chapter 4.

2.2 Fuel Thermal Conductivity Model Comparisons and Literature Review

CTF currently uses the MATPRO version 11 fuel thermal conductivity model from 1979 [1], which is a function of temperature, fractional density and composition of the fuel. The model is developed for unirradiated UO₂ and (U,Pu)O₂ fuels. The detailed model description can be found in Chapter 4.

On the other hand, FRAPCON-3.4 currently uses the modified NFI model [2], which includes the effects of exposure and gadolinia content. The fuel thermal conductivity calculation in FRAPCON first evolved from MATPRO model [3] and then it was updated with Lucuta’s model [4] which accounted for burnup degradation. However, there were some problems with Lucuta’s model. First, it predicted higher temperature values above 2200°K for unirradiated fuel pellets. Second, it couldn’t predict the burnup degradation effect on thermal conductivity above burnup levels ~30 GWd/MTU and thus had a non-conservative prediction when compared to the
high burnup pellet samples. The other drawback of Lucuta’s model was that the equation was non-standard such that it was not in the simple $1/(A+BT)$ form and it contained fitting multipliers for each factor (dissolved fission gas products, precipitated fission products, Maxwell porosity effect, radiation effects); therefore, it was difficult to make comparisons to other thermal conductivity models. Because of all these drawbacks, the Nuclear Fuels Industries thermal conductivity model developed by Ohira and Itegaki [5] was incorporated into FRAPCON-3 to replace the Lucuta’s model [2,4]. Some modifications were made to the original NFI model for burnup function in the phonon term and also in the electronic term. In addition to that, to capture the effect of the gadolinium addition to the fuel, an adjustment factor, which was developed by Massih et al. [6], was added to the denominator of the phonon term. Since all these modifications are done to the original NFI model, it is called “Modified NFI Model”, which incorporates both the burnup and gadolinium effects. Detailed model descriptions with the equations can be found in Chapter 4. Summary of the models can be found in Table 2-1.

Massih, A.R. et al. (1992) [6], developed a thermal conductivity model for unirradiated fuel considering the effects of gadolinium concentration and temperature. The model was compared against the experimental data and gave a very good agreement. In addition to that, a new fission gas release correlation was developed for irradiated (U,Gd)O$_2$ rods. The new fission gas release correlation is incorporated into the STAV-6 [6] fuel performance code. The calculated fission gas products release was compared against the experimental data from ABB Atom built BWRs irradiated up to 42 MWd/kgU with Gd concentration between 2 to 5wt %. The comparison of the results showed a good agreement between the predicted and measured fission gas release.

Lucuta, et.al. (1996) [4], published one of the most widely cited reference studies on the fuel thermal conductivity of irradiated UO$_2$ fuel. They investigated the thermal conductivity of
the irradiated UO₂ fuel considering the effects of burnup (dissolved and precipitated solid fission products), porosity, fission gas bubbles, deviation from stoichiometry, and radiation damage. All these factors are included into the correlation developed for irradiated UO₂. They also validated the correlation against available published data of SIMFUEL (Simulated Extended Burnup UO₂ Fuel) and radiation damage measurements. Lucuta’s model was recommended to be used below 1900°K. Sensitivity analyses were performed for different burnup levels from 1at. % burnup to 10at. % burnup levels as a function of temperature. It was observed that the reduction in the thermal conductivity was significant, especially in the low-temperature region of the fuel where radiation damage occurs. There is a large reduction in the predicted thermal conductivity in the 600°K to 700°K temperature range at extended burnup. For the higher temperature region, above 1500°K, the model shows no significant reduction over 56,000 MWd/t burnup level. Validation of the predicted thermal conductivities was made against the experimental data from Chalk River, Bettis, HBC (High Burnup Chemistry Club), JAERI (Japan Atomic Energy Research Institute), and AEA (Atomic Energy Authority) Technology and showed reasonable agreement.

Ohira K., and Itagaki N. (1997) [5] studied the thermal conductivity of high burnup UO₂ fuel pellet which was irradiated to 61 GWd/t in a commercial BWR. The measured data demonstrated that thermal conductivity degradation was higher than the SIMFUEL, which only included the effects of fission products under 1300°K. The results from the thermal conductivity data also showed that there was a thermal recovery effect above 1700°K. The recovery mechanism was explained by the migration of the vacancies. A new thermal conductivity model was developed considering the effects of not only the fission products but also the irradiation induced defects which had both accumulated defects and the recovery of these defects. The new model was incorporated into a fuel performance code and the fuel centerline temperatures were compared against the measured data from RISØ National Laboratory. The comparison of the fuel
centerline temperatures showed that results agreed within ± 150°C in the burnup range 15-50 GWd/t.

Sontheimer F., Ladskron H., and Billaux M.R. (1998) [7] developed a new fuel thermal conductivity correlation for UO₂ and UO₂-Gd₂O₃ fuels considering the effects of irradiation due to dissolving and precipitation of fission products in the fuel matrix, Oxygen-to-Metal (O/M) ratio change, bubble formation and irradiation damage accumulation and doping of UO₂ fuel with gadolinia. The new correlation was developed based on the relaxation-time theory of Klemens, which has a phonon term of the form of $\frac{1}{x} \arctan(x)$, where $x$ is the measure of the defect concentration introduced by burnup and gadolinia additions. Thermal conductivity predictions were compared against Halden data base [8] and it showed a very good agreement up to 40 GWd/kgU. Comparison of the new model for the cases with unirradiated UO₂/Gd₂O₃ fuel with up to 9 w/o Gd₂O₃ to the Siemens fuel thermal conductivity data [7] also showed a good agreement. Slight deviations were observed at 9 w/o Gd₂O₃. Arctan formulation is compared against the measurements from Ultra Halden High Burnup (UHB) experiments with burnup above 80 MWd/kgU for IFA-562 rod taking into account the pellet rim effects. Comparison of the results yielded a good agreement with experimental data whereas the classical form of thermal conductivity equation overpredicted the fuel centerline temperatures nearly 100°K.

Ronchi, et al. (1999) [9] studied the thermal conductivity of UO₂ between 500°K to 2900°K from the direct and simultaneous measurements of heat capacity and thermal diffusivity with an advanced laser-flash technique. It was observed that heat capacity continued to increase above 2670°K and thermal diffusivity showed a continuous net decrease with temperature up to 2400°K-2600°K. The measured heat capacity up to 2600-2700°K was in a good agreement with the present recommendations in the literature. Thermal diffusivity values were in a good
agreement up to 2200°K with the recommended values in the literature; however at higher temperatures, it was 30% lower than the assumed values in the literature.

Another study in the area of high burnup fuel behavior was performed by Motoe, S. (2000) [10]. The author focused on incorporating of a thermal conductivity degradation model for high burnup fuel into FEMAXI–IV [11], which was originally developed to analyze the thermal and mechanical behavior of light water fuel rods during steady and transient conditions as a function of reactor operating history. Halden reactor irradiated fuel rods IFA-519.9 were used to compare with experimental data against the updated code predictions for the range of 25–93 MWd/kg UO2. The three empirical models, Wiesenack [12], Ohira [5], and Lucuta [4], of fuel thermal conductivity were used in the study for the comparison purposes and to determine best prediction capabilities. As part of sensitivity analysis, fuel thermal conductivities were compared at two temperature levels (1000°K and 1600°K) for the burnup range varying from 0 to 100 MWd/kg UO2. In addition, peak centerline temperatures were also compared against the Halden experimental data for two rods and the results favored the Wiesenack’s model for better agreement with the data compare to other models. It was concluded that fission gas release is a function of the pellet temperature, which is more sensitive to the models of the thermal conductivity and the swelling rate of fuel. Hence, better prediction capabilities of these parameters are needed to evaluate fuel behavior in the high burnup region.

Minato, et al. (2001) [13] investigated thermal conductivities of both unirradiated and irradiated UO2 and UO2-Gd2O3 fuels. Disk-shaped samples with up to 10 w/o Gd2O3 were used to measure the thermal diffusivities by laser flash method from room temperature to about 1800°K. The experiments used uniform burnup distribution within each sample and thermal conductivities were calculated using thermal diffusivities, densities and specific heat capacity. Thermal conductivities of unirradiated UO2 and UO2-10 w/o Gd2O3 samples were measured and compared
against the models from MATPRO-11 [1], Harding and Martin [14] and the experimental data by Hirai and Ishimoto [15]. It was demonstrated that the measured data was slightly higher than the predicted values by MATPRO-11 and Harding and Martin but agreed well with the experimental data reported by Hirai and Ishimoto and also Lucuta et al [4]. Thermal conductivities of irradiated UO₂ and UO₂-10 w/o Gd₂O₃ samples were also measured and compared against the model proposed by Hirai et al. Comparison of the results gave good agreement with the experimental data. Model proposed by Hirai et al. assumes thermal conductivity degrades by fission products dissolved in the UO₂ matrix, irradiation-induced point defects with recovery completely above 1100°C and microbubbles which grow above 1400°C. It was concluded that thermal conductivities were decreased by irradiation and then it recovered around 1800°C due to recovery of the irradiation induced point defects during the measurement. Measured results of the thermal conductivity were almost the same with the model proposed by Hirai et al., which takes into account the irradiation induced defects, soluble fission products and gadolininium content.

Ronchi et al. (2004) [16], studied the effect of burnup on the thermal conductivity of uranium dioxide fuel that was irradiated from 30 GWd/t to 100 GWd/t. The research investigated the recovery of thermal conductivity as a function of temperature considering the effects of soluble fission products, fission gas frozen in dynamical solution and radiation damage. Thermal diffusivity and specific heat of the fuel were measured at various burnup levels via shielded laser flash device at Joint Research Center, Institute of Transuranium Elements (JRC-ITU). They used several thousand measurements points to develop a correlation for thermal conductivity. The predicted values from the correlation for the coefficients A and B were compared against the experimental results and the comparison showed that results agreed within 5% for most of the samples. The thermal conductivity results from the developed model were compared against the Halden correlation. It was seen that the maximum discrepancy between the two models were less
than 5% at 90 GWd/t, and at 35 GWd/t Ronchi’s model was 10% lower than the Halden correlation. The authors concluded that the effective decrease of thermal conductivity during reactor-irradiation was: 1) atomically dispersed fission products, 2) irradiation and self-irradiation defects, 3) fission gas and volatile fission products dynamically frozen in the fuel during irradiation, and 4) fission gas precipitation and porosity evolution.

Lyon, W.F., et al. (2004) [17] discussed the recent development of the steady state capability of Electric Power Research Institute’s (EPRI’s) fuel performance code, FALCON. It was stated that MATPRO was the primary source for the material properties and behavioral models in the code and it was subjected to extensive upgrade efforts to extend models to higher burnup ranges and to incorporate the new models not available within MATPRO before. Fuel pellet relocation, densification, melting, swelling and fuel thermal conductivity models were upgraded in addition to fission gas release, pellet rim formation, radial power and burnup distribution and cladding creep phenomena predictions. The Nuclear Fuel Industries Research (NFIR) fuel thermal conductivity model is incorporated into FALCON to replace MATPRO model. NFIR model was revised with some modifications to include the effects of Gd on thermal conductivity. Fuel centerline temperature results from FALCON/MATPRO and FALCON/NFIR were compared against Halden test rod IFA 515.10 rod A1 data. It was observed that NFIR fuel thermal conductivity model provided much more accurate results for high burnup (~50-55 GWd/tu) UO₂ fuel when compared to experimental data than the modified MATPRO model previously used in FALCON. The new model worked also well when compared to the experimental data for unirradiated (U,Gd)O₂ fuel. However, it constantly underpredicted the thermal conductivities for irradiated (U,Gd)O₂ samples and could not capture the thermal conductivity degradation due to Gd. The model was calibrated to by using additional test data for irradiated (U,Gd)O₂ rods. It was confirmed that fuel centerline temperature predictions for
irradiated (U,Gd)O$_2$ rods were greatly improved. The study concluded that FALCON is a useful licensing and best estimate fuel analysis tool applicable to wide range of steady state and transient operational conditions.

Jahingir, M.D. et al. (2007) [18] summarized recent upgrades and development on high burnup fuel behavior modeling at Global Nuclear Fuel (GNF) and qualification of thermal and mechanical performance code, PRIME03. The paper discussed the high burnup models in PRIME03 to include the high burnup mechanisms such as high burnup structure (rim) formation at the pellet periphery, burnup dependency of fuel pellet thermal conductivity, zircaloy creep, fuel pellet relocation, and fuel pellet fission gas release. PRIME03 was qualified to provide accurate prediction capability for different operating conditions and dimensions with high burnup data. The goal was to incorporate PRIME03 model into GNF fuel rod design and licensing process. The fuel pellet thermal conductivity was modeled to consider the impacts of burnup, gadolinium and additive. The phonon contribution to thermal conductivity was modified to account for the defect concentration due to both burnup and gadolinia. The study also compared fuel centerline temperature predictions for a moderately high burnup test fuel rod against the measured fuel centerline temperatures over the burnup range from 0 to 60 GWd/MTU and demonstrated the reasonable agreement. It was also noted that more than 600 fuel rods test data was used for the qualification purposes and roughly more than half of the fuel rods were having average burnups of greater than 40 GWd/MTU in the qualification database.

Bernard M. (2010) [19] presented the study on the code development in TRACE for the fuel thermal conductivity. The U.S. NRC Office of Research developed TRACE as a reactor systems analysis code for light water reactors to perform independent alternate analysis. In TRACE 5.0, MATPRO Version 9 fuel thermal conductivity was replaced with the FRAPCON-3 Modified NFI Model. Two accident scenarios were selected to demonstrate the effect of the new
model on the peak fuel and clad temperatures. Double ended cold leg LOCA and Main Stream Line Break accident conditions were chosen to study the impact of the new fuel thermal conductivity model on peak fuel and cladding temperature. It was concluded that with the modified NFI model in place, cold leg accident is more severe in duration and temperature (50°F higher Peak Clad Temperature and 40 seconds longer time for core reflood). On the other hand, for the main steam line break accident scenario, the cooling caused little difference in the values for thermal conductivities and produced similar results. It was confirmed that scenarios containing greatly increasing fuel temperatures are better scenarios to investigate the impact of fuel thermal conductivity on peak clad temperature predictions.

McGrath M. (2011) [20] described the OECD/NEA (Organization for Economic Co-operation and Development/Nuclear Energy Agency) Halden Reactor Project Mission and its history by re-emphasizing the international co-operative effort signed in 1958. She summarized the main goals of fuel testing’s and experiments performed in the Halden reactor to determine the fuel safety and operational margins for use in design and licensing of fuel such as under relevant operational conditions (power uprates, high burnup, advanced water chemistry), under accident conditions (LOCA), fuels representative of current industry (UO₂, MOX, etc) and innovative fuel concepts.

Halden project provides huge amount of measurement data for thermal conductivity and pellet temperatures. Industry has been benefited from the experiments to validate and to improve fuel performance models. In this research, Halden data for sample fuel rods will be used to analyze the performance of thermal conductivity model against burnup, temperature, and gadolinia concentration for both codes FRAPCON-3.4 and PSU/RDFMG version of COBRA-TF. Therefore, Halden experiments are very important for validation purposes of thermal conductivity model within subchannel code PSU/RDFMG version of COBRA-TF.
Geelhood, K. (2011) [21] gave an overview of the most recent versions of U.S. NRC steady state FRAPCON-3.4 and transient FRAPTRAN-1.4 fuel performance codes. In his paper, he talked about the recent updates incorporated into the codes including updated material properties models, models for new fuel and cladding types, cladding finite element analysis capability and ability to perform uncertainty analysis. FRAPCON-3 is the fuel performance code which developed to predict the long-term burnup response of one single fuel rod on steady state conditions. FRAPTRAN is the fuel performance code developed to predict the response of a fuel rod in transient conditions. Code development work is performed by Pacific Northwest National Laboratory (PNNL) for U.S. NRC. Assessment of FRAPCON-3.4 was demonstrated on thermal conductivity predictions and fuel centerline temperature predictions and the results were compared against the data that was used to develop the model. Comparison of fuel centerline temperatures were made at BOL for UO\textsubscript{2} and as a function of burnup for UO\textsubscript{2}, MOX and UO\textsubscript{2-Gd\textsubscript{2}O\textsubscript{3}} and showed reasonable agreement with a standard deviation of 5%.

In a recent study, Sudjana et al. (2013) [22], investigated Rod Ejection Accident (REA) as a design basis Reactivity Initiated Accident (RIA) for PWRs with a multi-physics code package to evaluate the margins with respect to the U.S. NRC interim criteria [23]. The research focused on analyzing the high cladding temperature and PCMI (Pellet-Cladding Mechanical Interaction) failure phenomena. The authors coupled 3-D neutronic code, PANTHER with the system thermal hydraulic code RELAP5, and the sub-channel thermal-hydraulic code, COBRA-3C_TE with a link to the fuel rod thermal-mechanical code, FRAPTRAN as part of the multi physics code package. The PANTHER code was used first to evaluate the neutronic data and to identify the potentially limiting ejected rod configurations in terms of large ejected rod worth and local peaking factor at Hot Zero Power (HZP), Hot Full Power (HFP) conditions and BOL and End of Life (EOL) core states. Next, Coupled PANTHER/Cobra-3C_TE was used to calculate
the REA transients for the selected ejected rod configurations. The transient nuclear power and peaking factors of the limiting rods were then transferred to FRAPTRAN code. The FRAPTRAN calculations were initialized by using steady state fuel rod results from FRAPCON calculations. They studied 3-Loop Westinghouse PWR design with UO$_2$-Gd$_2$O$_3$ fuel assemblies in the fresh batch as a reference plant for the analysis purposes. They summarized the results of calculated maximum enthalpy rise for different REA accident states and observed that the new PCMI criterion (60 cal/g) was met based on coupled codes and uncertainty analysis with extra margin to criteria achieved. The same observation was not valid for the base reference analysis done by using both 1D-2D former methods, indicating the strong interest and need to develop REA methodology based on the coupled 3D codes and appropriate uncertainty analysis.

2.3 COBRA-TF (CTF) Background and History

The COBRA-TF (COolant Boiling in Rod Arrays-Two Fluid) computer code was originally developed in 1980s by the Battelle Northwest Laboratories under the sponsorship of the U.S. NRC as a reactor vessel module of the coupled code system COBRA/TRAC [24]. Since then, various academic and industrial organizations have adapted, further developed and modified the code in many directions. The version owned by the Pennsylvania State University (PSU) [25] originates from the code version modified in cooperation with the FLECHT SEASET program [26]. The PSU/RDFMG version of code was extensively used to educate and train students in the area of nuclear reactor thermal-hydraulic safety analyses. The theoretical models and the numerical calculation schemes of the code were substantially improved with recent studies (27). The code was subject to an extensive verification and validation program as part of OECD Benchmarks and was applied to variety of light water reactor (LWR) steady state and transient simulations [28,29,30,31,32,33,34].
The PSU/RDFMG version of COBRA-TF, CTF [25], is an advanced sub-channel code, which has the capability of three-field representation of two-phase flow model. In CTF it is possible to model any vertical one, two, or three-dimensional component in the reactor vessel. However, the components outside of the reactor core itself, such as pump or pressurizer are not included in the code capabilities. In addition to Cartesian coordinates, CTF was developed for use with subchannel coordinates for more complex or irregular geometries such as rod bundle thermal-hydraulic analysis [26]. Unlike in the Cartesian coordinates, fixed transverse coordinates are not used in subchannel formulation. Instead, “gaps” are defined to specify the transfer connections between subchannels and complete the multidimensional mesh of the region. With the help of defining all the gap regions by one transverse equation regardless of the gap orientation, the number of components in conservation equations is reduced to only two as, vertical and transverse [35].

CTF uses MATPRO-11 correlation [1] to calculate the fuel thermal conductivity which does not incorporate the impact of thermal conductivity degradation by burnup and gadolinium. The goal of this research is to incorporate the thermal conductivity degradation both by burnup and gadolinia into the CTF for better predicting fuel temperature distribution within subchannel analysis. This will improve the accuracy of CTF calculations for void profile during transient conditions and margin to Departure from Nuclear Boiling or Critical Power Calculations for the cases that use both gadolinium and exposed fuel rods.

2.4 FRAPCON-3.4 Steady State Fuel Performance Code

FRAPCON-3 [2,35,36,37] is a fuel performance code which calculates the steady-state response of light-water reactor fuel rods during long term burnup conditions. The code is written in Fortran 90 programming language and the source can be compiled on any development environment with a Fortran 90 compiler. FRAPCON-3 has been developed for the U.S. Nuclear
Regulatory Commission by Pacific Northwest National Laboratory to calculate steady-state fuel behavior at high burnup conditions. The FRAPCON-3 code performs steady-state fuel rod calculations and also generates initial input conditions for transient fuel rod analysis code FRAPTRAN. The code computes the temperature, pressure, and deformation of a fuel rod as a function of time and includes the following models: 1) heat conduction through fuel and cladding to the coolant; 2) cladding elastic and plastic deformation; 3) fuel-cladding mechanical interaction; 4) fission gas release from the fuel and rod internal pressure; and cladding oxidation. The code also has material properties, water properties, and heat transfer correlations [37].

FRAPCON-3 code uses single-channel coolant enthalpy rise model for the fuel rod thermal response calculations. The code also uses a finite difference approach in heat conduction model like RELAP5 and FRAPTRAN which use a variable mesh spacing to accommodate the power peaking at the pellet edge which occurs in high burnup fuel operations [37].

FRAPCON-3.4 has been validated for BWRs, PWRs, and heavy-water reactors. The fuels that have been validated are uranium dioxide (UO₂), mixed oxide fuel ((U,Pu)O₂), urania-gadolinia (UO₂-Gd₂O₃), and UO₂ with zirconium diboride (ZrB₂) coatings. The cladding types that have been validated are Zircolay-2, Zircaloy-4, M5, and ZIRLO. FRAPCON-3.4 can predict fuel and cladding temperature, rod internal pressure, fission gas release, cladding axial and hoop strain, and cladding corrosion and hydriding [37]. Table 2-1 summarizes the fuel thermal conductivity models used in CTF and FRAPCON-3.4.
### Table 2-1 Summary of Thermal Conductivity Equations

<table>
<thead>
<tr>
<th>Models</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTF MATPRO-11 (1979)</td>
<td>$k_{UO_2} = \left[ \max \left( 0.0191, \frac{40.4}{(T - 273.15) + 464.} \right) + 1.216 \times 10^{-4}e^{\left(1.867 \times 10^{-3}(T-273.15)\right)} \right] \times C$</td>
</tr>
<tr>
<td></td>
<td>Where</td>
</tr>
<tr>
<td></td>
<td>$k_{UO_2}$ = Fuel thermal conductivity, W/m·°K</td>
</tr>
<tr>
<td></td>
<td>$C = 100 \times \left[ \frac{1-\beta(1-f_D)}{1-0.05\beta} \right]$</td>
</tr>
<tr>
<td></td>
<td>$\beta = 2.58 - (5.8 \times 10^{-4})(T-273.15)$</td>
</tr>
<tr>
<td></td>
<td>$T$ = Temperature, °K</td>
</tr>
<tr>
<td></td>
<td>$f_D$ = Fuel Theoretical density</td>
</tr>
<tr>
<td>MATPRO-11 Rev.2 (1981)</td>
<td>$k_{UO_2} = \frac{D}{(1+(6.5-0.00469T'(1-D))/\left(\frac{C_v}{(A+BT'\times(1+3ethical))} + ... \right)\frac{5.2997 \times 10^{-3}T}{\exp(-13358/T)\times(1+0.169\times13358/T\times2)^2}}$</td>
</tr>
<tr>
<td></td>
<td>Where</td>
</tr>
<tr>
<td></td>
<td>$k_{UO_2}$ = thermal conductivity (W/m·°K)</td>
</tr>
<tr>
<td></td>
<td>$D$ = fraction of theoretical density (unitless)</td>
</tr>
<tr>
<td></td>
<td>$C_v$ = phonon contribution to the specific heat at constant volume (J/kg·°K). The first term of the correlation for fuel specific heat capacity is used for this factor.</td>
</tr>
<tr>
<td></td>
<td>$ethical$ = linear strain caused by thermal expansion when temperature is &gt;300°K (unitless). The MATPRO correlation for fuel thermal expansion is used for this factor.</td>
</tr>
<tr>
<td></td>
<td>$T$ = fuel temperature (°K)</td>
</tr>
<tr>
<td></td>
<td>$T' = porosity correction for temperature, T &lt; 1364°K, T' = 6.50 - T*(4.69 \times 10^{-3})$</td>
</tr>
<tr>
<td></td>
<td>$T' = -1$ if $T &gt; 1834°K$</td>
</tr>
<tr>
<td></td>
<td>$1364°K &lt; T &lt; 1834°K, T'$ is found by interpolation</td>
</tr>
<tr>
<td></td>
<td>$T''$ = fuel temperature if $T &lt; 1800°K$</td>
</tr>
<tr>
<td></td>
<td>$T'' = 2050°K$ if $T &gt; 2300°K$</td>
</tr>
<tr>
<td></td>
<td>$1800°K &lt; T &lt; 2300°K, T''$ is found by interpolation</td>
</tr>
<tr>
<td></td>
<td>$A$ = a factor proportional to the point defect contribution to the phonon mean free path (m-s/kg·°K), the correlation used for this factor is 0.339+12.6 * (absolute value (2.0-O/M ratio).</td>
</tr>
<tr>
<td></td>
<td>$B$ = a factor proportional to the phonon-phonon scattering contribution to the phonon mean free path (m-s/kg·°K); the correlation used for this factor is 0.0687 * (1+0.6238*plutonium content of the fuel).</td>
</tr>
<tr>
<td>Lucuta (1996)</td>
<td>$k_0 = \frac{1}{0.0375+2.165 \times 10^{-4}T} + \left[ \frac{4.715 \times 10^9}{T^2} \right] \exp \left[ -\frac{16361}{T} \right]$</td>
</tr>
<tr>
<td></td>
<td>Where</td>
</tr>
<tr>
<td></td>
<td>$k_0$ = thermal conductivity of unirradiated, fully dense urania (W/m·°K)</td>
</tr>
<tr>
<td></td>
<td>$T$ = temperature (°K)</td>
</tr>
<tr>
<td></td>
<td>$FD = \left[ \frac{1.09}{B^{1.265} + \frac{0.0643}{\sqrt{B}}} \right] \arctan \left[ \frac{1}{B^{1.265} + \frac{0.0643}{\sqrt{B}}} \right]$</td>
</tr>
<tr>
<td></td>
<td>Where</td>
</tr>
<tr>
<td></td>
<td>$T$ = temperature (°K)</td>
</tr>
<tr>
<td>Models</td>
<td>Equations</td>
</tr>
<tr>
<td>--------</td>
<td>-----------</td>
</tr>
<tr>
<td><strong>B=burnup in atom % (1% atom=9.383 GWd/MTU at 200 MeV/fission)</strong></td>
<td>[ FP=1+ \left( \frac{0.019B}{3 - 0.019B} \right) \left( \frac{1}{1 + \exp \left( \frac{1}{T - 1200} \right)} \right) ]</td>
</tr>
<tr>
<td></td>
<td>[ FM=\frac{1-p}{1+(s-1)p} ]</td>
</tr>
<tr>
<td>where;</td>
<td></td>
</tr>
<tr>
<td>P= porosity fraction (as fabricated plus swelling)</td>
<td></td>
</tr>
<tr>
<td>S=shape factor (=1.5 for spherical pores)</td>
<td></td>
</tr>
<tr>
<td>[ \text{FR}=1-\frac{0.2}{1+\exp\left(\frac{T-900}{80}\right)} ]</td>
<td></td>
</tr>
<tr>
<td>Ohira and Itagaki (1997)</td>
<td>[ k=K_0<em>FD</em>FP<em>FM</em>FR ]</td>
</tr>
<tr>
<td><strong>k</strong></td>
<td>[ k_{\text{Original NFI Model}}= \frac{1}{A+BT+f(Bu)+g(Bu)h(T)-CT^2+DT^4} ]</td>
</tr>
<tr>
<td><strong>k</strong></td>
<td>[ k_{\text{Mod. NFI Model}}= \frac{1}{A+a<em>gad+BT+f(Bu)+(1-0.9</em>\exp(-0.04Bu))*g(Bu)h(T)+E/\pi^2+\exp(-F/\pi)} ]</td>
</tr>
<tr>
<td>Where</td>
<td></td>
</tr>
<tr>
<td>( k_95 = \text{Thermal Conductivity for 95% dense fuel, W/m}^{-\circ}\text{K} )</td>
<td></td>
</tr>
<tr>
<td>T= Temperature, °K</td>
<td></td>
</tr>
<tr>
<td>Bu= Burnup, GWd/MTU</td>
<td></td>
</tr>
<tr>
<td>f(Bu)= Effect of fission products in crystal matrix (solution)=0.00187 * Bu</td>
<td></td>
</tr>
<tr>
<td>g(Bu)= Effect of irradiation defects</td>
<td></td>
</tr>
<tr>
<td>( = 0.038 * Bu^{0.28} )</td>
<td></td>
</tr>
<tr>
<td>h(T)= Temperature dependence of annealing on irradiation defects</td>
<td></td>
</tr>
<tr>
<td>[ h(T)=\frac{1}{1+396\exp(-Q/T)} ]</td>
<td></td>
</tr>
<tr>
<td>Q=Temperature dependent parameter =6380 °K</td>
<td></td>
</tr>
<tr>
<td>A= 0.0452 m°K/W</td>
<td></td>
</tr>
<tr>
<td>a= constant = 1.1599</td>
<td></td>
</tr>
<tr>
<td>gad= weight fraction of gadolinia</td>
<td></td>
</tr>
<tr>
<td>B=2.46 ( 10^{-4} ) m°K/W°K</td>
<td></td>
</tr>
<tr>
<td>E= 3.5 ( 10^{9} ) W°K/m</td>
<td></td>
</tr>
<tr>
<td>F= 16,361 °K</td>
<td></td>
</tr>
<tr>
<td>( k_d=1.0789<em>k_95</em>d )</td>
<td></td>
</tr>
<tr>
<td>Where</td>
<td></td>
</tr>
<tr>
<td>d = density in fraction of TD</td>
<td></td>
</tr>
<tr>
<td>( k_95 = \text{as given conductivity based on 95%TD.} )</td>
<td></td>
</tr>
<tr>
<td>( k_d = \text{thermal conductivity adjusted for as fabricated fuel density,d.} )</td>
<td></td>
</tr>
<tr>
<td>1.789 ( \text{the adjustment factor for conductivity at 100% TD.} )</td>
<td></td>
</tr>
</tbody>
</table>
2.5 Physical Mechanisms Occurring in The Fuel Rod During High Burnup

The extended fuel operations with high burnup causes some changes in the fuel and cladding structure that affect the fuel mechanical and thermal performance. These changes occur in the fuel and cladding due to the prolonged irradiation, corroding environment and high temperature in the reactor core. The microstructure of the fuel and cladding changes in the reactor due to many factors: irradiation damage, high temperature, mechanical stresses and chemical reactions [38]. The most important degradation mechanisms occurring in the fuel cladding during high burnup operations are summarized in the following sections.

2.5.1 Cladding Degradation Mechanisms During High Burnup

The main cladding degradation mechanisms during high burnup are uniform waterside corrosion, hydriding and radiation damage.

**Uniform waterside corrosion** occurs on the outer surface of cladding during reactor operation. The zirconium in cladding chemically reacts with the water flowing around the cladding as coolant, developing a protective oxide on the surface of the cladding. The rate of corrosion is determined by many factors such as irradiation temperature, radiation-induced changes to cladding microchemistry, coolant chemistry, alloy chemistry and thermo-mechanical treatment. For fuel burnups greater than 50 GWd/t, the oxide thickness can exceed 100 µm depending on fuel duty. All of the zirconium alloys studied so far indicates a change in corrosion rate when oxide thickness exceeds 20-30 µm. If the cladding has a large oxide thickness, the oxide layer may detach and break off, which is called oxide spalling. Oxide spalling causes a thinner oxide layer which creates a cold spot and may start hydride blister formation. All of these changes affect cladding ductility and cladding thermal conductivity [38]. In addition, crud deposition may occur on the outer surface of the cladding due to the buildup of reactor water corrosion products.
Both cladding oxidation and crud deposition provide additional heat transfer resistance and increase the cladding and fuel temperatures. However, they are not the limiting thermal resistances affecting the fuel centerline temperature.

**Hydriding** occurs when hydrogen generated by the corrosion reaction precipitates as zirconium hydride throughout the cladding thickness when corrosion layer thickness exceeds 50 µm.

\[
\text{Zr} + 2 \text{H}_2\text{O} \rightarrow \text{ZrO}_2 + 2\text{H}_2 \text{ (gas)}
\]

Approximately 15%-20% of the hydrogen produced by the corrosion reaction is absorbed into the alloy. When hydrogen level is greater than 1000 ppm, the cladding becomes brittle. Lower hydrogen levels (600-800 ppm) can also have an impact on cladding ductility at lower temperatures and can also degrade the overall cladding ductility, depending on the hydride distribution. The main problem with hydriding is that hydrides are brittle and lower cladding ductility. In addition to that, hydride may create weak spots in the cladding due to the formation of a hydride rim or hydride blister [38].

**Radiation damage** causes mechanical and geometrical properties of the material to change as a result of microstructural defects. An energetic particle (e.g. neutron or fission fragment) strikes with an atom in a material, transferring some of its energy to the atom and knocking it out of its lattice position. The knock-on atom and the recoiling particle make additional collisions with other atoms generating a cascade of displaced atoms. Knowing that the energy of a fission neutron is ~2 MeV, a PKA (primary knock on atom) energy up to ~ 40 KeV can be created, given that the threshold energy to displace an atom from its lattice position in metals is ~20–40 eV. A typical number of displaced atoms in a displacement cascade is ~500.
In most metals, 90–99% of these displaced atoms eventually come back to lattice positions. The annihilation process may cause the formation of defect cluster, causing hardening, swelling and creep.

Macroscopic changes are the observable physical changes in material properties such as embrittlement, radiation induced growth and swelling, creep which change the geometry of the cladding. When fuel burnup reaches 30 GWd/t, cladding has suffered about 20 dpa (displacements per atom) which means that each atom is going to be displaced 20 times from its location in the crystal lattice structure. The amount of dpa is proportional to burnup [38].

The main issue with radiation damage in the cladding is that it causes radiation hardening (yield stress increases while uniform strain decreases and hardening increases and ductility decreases), change of corrosion resistance through micro-chemical changes, mechanical property changes and deformation localization (e.g., dislocation channeling, possibly leading to easier axial crack propagation) [38].
2.5.2 Fuel Pellet Degradation Mechanisms During High Burnup

Fission gas is formed inside the UO₂ fuel pellet during normal reactor operations and can be found in the fuel as follows [38]:

1) Gas dissolved in the UO₂ matrix
2) Gas in intragranular bubbles (matrix)
3) Gas in intragranular bubbles (on grain boundaries)
4) Gas released to rod void volume
5) Gas in fuel porosity

Since the solubility of fission gases in UO₂ is low, the amount of the gas dissolved in the UO₂ matrix is small. Gas in intragranular bubbles (matrix) and on grain boundaries causes fuel swelling resulting in pellet-cladding mechanical interaction (PCMI). Gas released to rod void volume occurs due to the fission gas release (FGR) which results in an increase in internal rod pressure and hoop stresses on cladding. The distribution of fission gas in the fuel depends on power history, temperature and fuel microstructure [38].

The physical mechanisms occurred in the fuel pellet are summarized as follows:

**Rim Formation** is the micro-structural evolution which occurs at high burnups on the fuel pellet periphery. It is formed near the outer surface (rim) of UO₂ fuel pellets where the burnup is highest because of the resonance neutron capture by $^{238}\text{U}$ forming fissile $^{239}\text{Pu}$. The region is called rim region and its thickness is around 100-300 µm. Rim region is formed when the local fuel rod burnup exceeds 60 GWd/t. It is characterized by sub-micrometer-size grains with bubbles. Formation of the rim structure increases porosity on the pellet periphery around 10%-20% which causes a decrease in thermal conductivity and an increase in fuel temperature in that region [38]. Rim structure formation affects thermal behavior, fission gas release and PCI behavior under normal and transient conditions [43].
**Micro-cracking** occurs during high burnup operations since the as-fabricated grain boundaries become brittle from the precipitation of fission gas bubbles and solid fission products. In addition to that it is also induced by overpressurization of intergranular fission bubbles or coarsened rim bubbles during a sudden relief of PCMI restraints by cladding or a rapid increase of temperature such as power transient, reactivity initiated accident (RIA) and loss-of-coolant accident (LOCA) [43]. The micro-cracking can have an impact on fission gas swelling and deformation [38].

**Pellet Cladding Interaction** occurs during high burnup operations. As burnup increases, a metallurgical and chemical bond starts to form between the cladding and the fuel. Fuel-cladding bonding is established when clad-fuel contact occurs as a result of cladding creep down and fuel swelling [38]. Fission gas release and swelling has an impact on PCI [43].

### 2.6 Mechanisms of Thermal Conductivity Degradation During High Burnup

Thermal conductivity of irradiated UO$_2$ is affected by the changes that take place in the fuel during irradiation: solid fission product build up, porosity and fission gas bubble formation, and radiation damage [4,39].

a) **Solid Fission Product Build Up:** Fission products are generated in the fuel as a result of fission reaction.

Kleykamp [40] grouped fission products as follows:

- Gases and other volatile elements: Br, Kr, Rb, I, Xe, Cs, Te.
- Metallic precipitates: Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Se, Te.
- Oxide precipitates: Rb, Sr, Zr, Nb, Mo, Se, Te, Cs, Ba.
- Dissolved as oxides in the fuel matrix: Rb, Sr, Y, Zr, Nb, La, Ce, Pr, Nd, Pm, Sm, Eu.
The solid fission products formed during irradiation (dissolved and precipitated) has an impact on the fuel thermal conductivity by changing the fuel lattice structure. Several studies have been made theoretically or experimentally to evaluate the effect of the fission products on thermal conductivity. It was shown that the dissolved fission products lower the thermal conductivity, whereas the precipitated fission products increase the thermal conductivity of UO₂ due to the higher thermal conductivity of metallic precipitates than UO₂ matrix [4,39].

b) **Irradiation Defects:** Radiation damage generates additional defects in the fluorite lattice especially in the cold regions of the fuel at temperatures below 1100°K. At higher temperatures the defects from radiation damage are annealed. Radiation damage from neutrons, alpha decay and fission increases the number of lattice defects and as a result reduce the thermal conductivity of the fuel [4,39].

c) **Porosity Increase Due to Rim Formation:** In high burnup fuel operations, a microstructural evolution is developed at the fuel pellet periphery called rim structure. It increases the porosity resulting in a decrease the fuel thermal conductivity on the pellet periphery and therefore an increase in the fuel temperature [39].

d) **Impurities and Additives:** Impurities or additives in UO₂ decrease thermal conductivity like fission products. Thermal conductivity of UO₂/Gd₂O₃ decreases with the amount of Gd₂O₃. Gd₂O₃ has a body centered cubic structure and therefore it may deform lattice structure of UO₂ which has a face-center cubic structure. In addition, Gd₂O₃ has an impact on phonon-phonon scattering characteristic due to the mass difference between Gd₂O₃ and UO₂ [39].
2.7 References


42. “Development of Radiation resistant Reactor Core Structural Materials”,
   http://www.iaea.org/About/Policy/GC/GC51/GC51InfDocuments/English/ge51inf-3-att7_en.pdf

CHAPTER 3
SENSITIVITY ANALYSIS OF BWR FUEL ROD THERMAL PROFILE

3.1 Introduction

This section covers the sensitivity study performed to investigate the radial fuel rod thermal behavior. Four fuel rod parameters – fuel thermal conductivity, gap conductance, fuel pellet radius, and clad inside radius - were selected and effect of each parameter on the fuel rod radial temperature profile was investigated. Three power levels (16.4, 32.8 and 49.2 kW/m) were used to simulate a typical BWR fuel rod operating condition.

The reason for conducting this sensitivity study is to identify the relationship and impact between the radial fuel temperature behavior and each fuel parameter and to determine the critical few factors. Each fuel parameter has an effect on the fuel rod temperature profile representing fuel physical phenomena such as fuel cracking, fuel relocation, fuel swelling, fuel creep down and clad creep down occurring during a typical reactor operation. Results from this study are going to give us clear understanding of effect of each parameter on the fuel rod temperature profile.

The motivation for this study is to improve the prediction capability and reduce the uncertainties in the fuel rod temperature calculations of CTF. It will help us to understand which fuel parameter will have the dominant effect on the radial fuel temperature profile based on the analytical solution of the conduction equation across the fuel rod. The analysis results will be used as guidance when improving the fuel rod models in CTF and the sensitivity results will provide us an idea on which fuel parameter has the dominant effect to reduce the uncertainties in the fuel temperature predictions in a typical fuel rod operating conditions. This study will also demonstrate us the potential benefits of improving the model accuracies in CTF.
3.2 Analytical Solution to Cylindrical Fuel Rod Radial Temperature Profile

The analytical solution [1] for a cylindrical fuel rod radial temperature profile is used to calculate the temperature drop between the fuel centerline and the coolant temperature, and it is a function of both linear heat generation rate and the thermal resistance term. The overall thermal resistance for a cylindrical fuel pin is demonstrated in Figure 3-1.

Temperature drop across the fuel pellet is predicted from Equation 3-1:

\[ T_{\text{max}} - T_{f0} = \frac{q'}{4\pi k_f} \]  
Equation (3-1)

Temperature drop across the gap is given by Equation 3-2:

\[ T_{f0} - T_{ci} = \frac{q'}{2\pi R_g h_g} \]  
Equation (3-2)

Temperature drop across the cladding is given by Equation 3-3:

\[ T_{ci} - T_{co} = \frac{q'}{2\pi k_c} \ln \left( \frac{R_{co}}{R_{ci}} \right) \]  
Equation (3-3)

Temperature drop between the clad outside and bulk temperature is given by Equation 3-4:

\[ T_{co} - T_m = \frac{q'}{2\pi R_{co} h} \]  
Equation (3-4)

The overall resistance across the fuel rod is given by Equation 3-5:

\[ T_{\text{max}} - T_m = q' \left[ \frac{1}{4\pi k_f} + \frac{1}{2\pi R_g h_g} + \frac{1}{2\pi k_c} \ln \left( \frac{R_{co}}{R_{ci}} \right) + \frac{1}{2\pi R_{co} h} \right] \]  
Equation (3-5)

Where;

- \( T_{\text{max}} \)= Fuel center line temperature, °K
- \( T_{ci} \)= Clad inside temperature, °K
- \( T_m \)= Mean coolant temperature, °K
- \( q' \)= Linear Heat Generation rate, W/m
- \( k_f \)= Fuel average thermal conductivity, W/m°C
- \( R_g \)= Mean gap radius, \((R_{co}+R_{ci})/2\), m
- \( h_g \)= Effective gap conductance, W/m²°C
T_{co} = Clad outside temperature, °K
R_{co} = Clad outside radius, m
R_{ci} = Clad inside radius, m
k_{c} = Cladding thermal conductivity, W/m-°K
h = Heat transfer coefficient of the coolant, W/m^{2}.°K

3.3 Sensitivity Study

Sensitivity study was performed for the four fuel parameters: fuel thermal conductivity, gap conductance, fuel pellet radius, and clad inside radius. The reason why heat transfer coefficient of the coolant was not included in these sensitivity parameters is that nuclear boiling water heat transfer coefficient is so large and therefore the effect on the delta temperature will be so small and it will have no effect on the fuel centerline temperature.

An analytical solution to the general conduction equation for the fuel rod radial temperature behavior was used in this study. The operating domain for each parameter was selected to simulate the typical BWR bundle operating conditions. A hundred and thirty-two (132) test points were created using three different linear heat generation rates: 16.4, 32.8, and 49.2 kW/m referring to 5, 10 and 15 kW/ft respectively.
First fuel thermal conductivity was changed and the other three parameters: gap conductance, fuel pellet radius and clad inside radius were kept constant, then the next parameter was changed, and the other three were kept at the reference point values. The reference test point values for each parameter are given in Table 3-1 and test matrix operating domain for each parameter is given in Table 3-2.

Table 3-1 Reference Test Case Values Used at Each Power Level

<table>
<thead>
<tr>
<th>Fuel Thermal Conductivity $k_f$ (W/m-K)</th>
<th>Gap Conductance $h_g$ (W/m²-K)</th>
<th>Fuel Pellet Radius $R_{fo}$ (m)</th>
<th>Clad Inside Radius $R_{ci}$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
</tbody>
</table>

Table 3-2 Operating Domain for Each Parameter used in the Sensitivity Analysis Test Matrix

<table>
<thead>
<tr>
<th>Linear Heat Generation Rate $q'$ (kW/m)</th>
<th>Fuel Thermal Conductivity $k_f$ (W/m-°K)</th>
<th>Gap Conductance $h_g$ (W/m²-°K)</th>
<th>Fuel Pellet Radius $R_{fo}$ (m)</th>
<th>Clad Inside Radius $R_{ci}$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.4</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>32.8</td>
<td>2.8</td>
<td>10000</td>
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</tr>
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<td>49.2</td>
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<td>0.00612</td>
</tr>
<tr>
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</tr>
<tr>
<td></td>
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<td>0.00606</td>
</tr>
<tr>
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<td>2.6</td>
<td>35000</td>
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</tr>
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<td>0.00677</td>
</tr>
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<td></td>
<td>2.3</td>
<td>50000</td>
<td>0.00594</td>
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<td>2.2</td>
<td>55000</td>
<td>0.00591</td>
<td>0.00715</td>
</tr>
</tbody>
</table>
3.4 Fuel Thermal Conductivity

Effect of fuel thermal conductivity on the fuel radial temperature were investigated for different power levels. Fuel thermal conductivity was changed for each linear heat generation rate keeping the other three fuel parameters constant. It was observed that as the thermal conductivity decreased, the fuel temperature increased and the maximum increase occurred at the fuel center line. The clad inside and, outside temperatures and the gap temperature did not see a significant effect by the change in the fuel thermal conductivity. As the fuel thermal conductivity increased, fuel temperature decreased as expected. In general $k(T)$ decreases with increasing temperature.

As the fuel thermal conductivity decreased, the maximum temperature deviation from the reference test case was observed in the fuel centerline and the deviation increased as the power level increased. The maximum increase in temperature from the reference test case was 14.0 % at $q' = 49.2 \text{ kW/m}$. 

As the fuel thermal conductivity increased, the fuel temperature decreased. The maximum deviation in the fuel temperature from the reference test point occurred in the fuel centerline and the deviation increases as the power level increases. The maximum decrease was 9.6 % at $q' = 49.2 \text{ kW/m}$. 

The physical phenomena behind fuel thermal conductivity decrease could be the fuel cracking, the fuel expansion and the fuel swelling and fission gas release mechanism related. The physical phenomena behind fuel conductivity increase could be fuel densification, loss of the pores in the fuel structure and increase of the gap width and resulting in a increase in gap conductance.
Figure 3-2 through Figure 3-8 are summarizing the results for the fuel thermal conductivity effect. At each power level, eleven (11) test points were simulated and the values for each parameter were tabulated in Table 3-4 below.

Table 3-4 Test Points used at Each Power Level

<table>
<thead>
<tr>
<th>Test Number</th>
<th>Fuel Thermal Conductivity (W/m·ºK)</th>
<th>Gap Conductance (W/m²·ºK)</th>
<th>Fuel Pellet Radius (m)</th>
<th>Clad Inside Radius (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>2</td>
<td>2.8</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>3</td>
<td>2.9</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>4</td>
<td>3.0</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>5</td>
<td>3.1</td>
<td>4300</td>
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<td>0.00621</td>
</tr>
<tr>
<td>6</td>
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<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>7</td>
<td>2.6</td>
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<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>8</td>
<td>2.5</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>9</td>
<td>2.4</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>10</td>
<td>2.3</td>
<td>4300</td>
<td>0.00606</td>
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<tr>
<td>11</td>
<td>2.2</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
</tbody>
</table>

Table 3-5 Maximum Radial Temperature Deviation at Each Power Level

<table>
<thead>
<tr>
<th>Power Level q' (kW/m)</th>
<th>Maximum radial temperature (ºK) deviation from the reference test case</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Increase (%)</td>
</tr>
<tr>
<td>16.4</td>
<td>9.5</td>
</tr>
<tr>
<td>32.8</td>
<td>12.5</td>
</tr>
<tr>
<td>49.2</td>
<td>14.0</td>
</tr>
</tbody>
</table>
Figure 3-2 Radial Fuel Temperature Profile for a BWR Rod using Different Fuel Thermal Conductivity Values at $q' = 16.4$ kW/m

Figure 3-3 Radial Fuel Temperature Profile for a BWR Rod using Different Fuel Thermal Conductivity Values at $q' = 32.8$ kW/m
Figure 3-4 Radial Fuel Temperature Profile for a BWR Rod using Different Fuel Thermal Conductivity Values at $q' = 49.2 \text{ kW/m}$

Figure 3-5 Radial Fuel Temperature Deviation Profile from the BWR Reference Test Case at $q' = 16.4 \text{ kW/m}$
Figure 3-6 Radial Fuel Temperature Deviation Profile from the BWR Reference Test Case at $q' = 32.8$ kW/m

Figure 3-7 Radial Fuel Temperature Deviation Profile from the BWR Reference Test Case at $q' = 49.2$ kW/m
In order to simulate the effect of the gap conductance on the fuel rod temperature profile, the gap conductance was increased from the reference point 4300 W/m²·°K to 55,000 W/m²·°K. Eleven (11) test points were created for each power level and the values for each parameter are tabulated in Table 3-6 below. The radial fuel rod temperature profiles across the fuel radius at different power levels are shown in Figure 3-9 through Figure 3-11. It is seen that as the gap conductance increased, the fuel temperature decreased.

In a typical BWR fuel rod operation, during burnup with the combination of the fuel relocation, the fuel expansion, and the cladding creep down the gap thickness decreases and the fuel-clad interaction occurs resulting in an increase in the gap conductance. As the gap
conductance increases, the thermal resistance between the fuel and the clad is reduced resulting in an enhanced heat removal from the fuel and finally a reduction in the fuel rod temperature across the fuel pellet radius. The shape of the fuel temperature profile is independent of the gap conductance; however, the amount of the decrease in temperature is dependent on the gap conductance. The maximum decrease in the fuel rod temperature is observed when the gap conductance, \( h_g \), is between 10,000 and 20,000 W/m\(^2\)-ºK. For the test cases with \( h_g > 20,000 \) W/m\(^2\)-ºK, the fuel rod temperature did not see a significant change.

Figure 3-12 through Figure 3-14 show that the temperature decrease, \( \Delta T \), across the fuel pellet centerline, the midpoint, and the surface is the same. The maximum decrease from the reference test point is seen when \( h_g = 10,000 \) W/m\(^2\)-ºK. As \( h_g \) is increased above 20,000 W/m\(^2\)-ºK, the decrease in the \( \Delta T \) was not significant. Figure 3-15 shows the fuel centerline temperature versus the gap conductance at different power levels. The reference gap conductance is chosen as 4300 W/m\(^2\)-ºK. It is seen from the regression coefficient \( R^2 = 0.58 \) that there is no strong linear relationship between the gap conductance and the fuel centerline temperature. As the power level increased, the fuel centerline temperature increased.

**Table 3-6** Test Points used at Each Power level

<table>
<thead>
<tr>
<th>Test Number</th>
<th>Fuel Thermal Conductivity (W/m-ºK)</th>
<th>Gap Conductance (W/m(^2)-ºK)</th>
<th>Fuel Pellet Radius (m)</th>
<th>Clad Inside Radius (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>2</td>
<td>2.7</td>
<td>10000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>3</td>
<td>2.7</td>
<td>15000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>4</td>
<td>2.7</td>
<td>20000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>5</td>
<td>2.7</td>
<td>25000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>6</td>
<td>2.7</td>
<td>30000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>7</td>
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<td>35000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>8</td>
<td>2.7</td>
<td>40000</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>9</td>
<td>2.7</td>
<td>45000</td>
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<td>0.00621</td>
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</table>
Table 3-7 Percent (%) Temperature Drop (delta T) from the Reference Case at Each Power Level

<table>
<thead>
<tr>
<th>% deltaT</th>
<th>q' (kW/m)</th>
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</thead>
<tbody>
<tr>
<td>-7.9</td>
<td>16.4</td>
</tr>
<tr>
<td>-10.4</td>
<td>33.8</td>
</tr>
<tr>
<td>-11.6</td>
<td>49.2</td>
</tr>
</tbody>
</table>

Table 3-8 Temperature Drop (deltaT) from the Reference Case at Each Power Level for Different Gap Conductance Values

<table>
<thead>
<tr>
<th>deltaT (°K)</th>
<th>q'=16.4 kW/m</th>
<th>q'= 33.8 kW/m</th>
<th>q'= 49.2 kW/m</th>
<th>hg (W/m²·°K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-56.4</td>
<td>-112.8</td>
<td>-169.3</td>
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<td></td>
</tr>
<tr>
<td>-70.6</td>
<td>-141.2</td>
<td>-211.8</td>
<td>15000</td>
<td></td>
</tr>
<tr>
<td>-77.7</td>
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<td>-233.1</td>
<td>20000</td>
<td></td>
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</table>

Table 3-9 Fuel Centerline Temperature at Different Power Levels

<table>
<thead>
<tr>
<th>Linear Heat Generation Rate</th>
<th>Fuel Centerline (°K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>q' (kW/m)</td>
<td>hg= 4300 (W/m²·°K)</td>
</tr>
<tr>
<td>16.4</td>
<td>1154</td>
</tr>
<tr>
<td>33.8</td>
<td>1758</td>
</tr>
<tr>
<td>49.2</td>
<td>2362</td>
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</tbody>
</table>
Figure 3-9 Radial Temperature Profile for a BWR Rod with Changing the Gap Conductance at $q' = 16.4$ kW/m

Figure 3-10 Radial Temperature Profile for a BWR Rod with Changing the Gap Conductance at $q' = 32.8$ kW/m
Figure 3-11 Radial Temperature Profile for a BWR Rod with Changing the Gap Conductance at $q' = 49.2$ kW/m

Figure 3-12 Radial Temperature Deviation Profile from the BWR Reference Test Case by Changing Gap Conductance at $q' = 16.4$ kW/m
Figure 3-13 Radial Temperature Deviation Profile from the BWR Reference Test Case by Changing Gap Conductance at \( q' = 32.8 \text{ kW/m} \)

Figure 3-14 Radial Temperature Deviation Profile from the BWR Reference Test Case by Changing Gap Conductance at \( q' = 49.2 \text{ kW/m} \)
3.6 Fuel Pellet Radius

The effect of the fuel pellet radius on the fuel temperature profile was investigated at three different power levels: 16.4, 32.8, and 49.2 kW/m. Total of eleven (11) test points tabulated in Table 3-11 below were calculated at each power level to simulate the effect of the change in the fuel pellet radius on the fuel rod temperature profile. Figures 3-16, 3-17 and 3-18 show the fuel rod temperature profile at three different power levels. It is seen from these figures that as the fuel radius increased the fuel temperature in the middle and towards the surface of the fuel pellet also increased. The fuel centerline, the clad inside and outside temperature, and the bulk temperature did not see a significant change with the change in the fuel pellet radius. As the power increased from 16.4 kW/m to 49.2 kW/m, the fuel centerline temperature also increased. Table 3-10 below summarizes the fuel centerline temperature at each power level.
Figures 3-19, 3-20, and 3-21 show the amount of the deviation in the fuel temperature, \( \delta T \), from the reference test case (Test number 1). It is seen from these figures that change in \( \delta T \) is the same across the fuel pellet and increased as the power level increased. The maximum deviation was 0.6 \% compared to the reference test case. This concludes that changing the fuel pellet radius does not show much change in the fuel temperature. As the fuel radius is decreased, gap between the fuel pellet and the clad is increased resulting in an increase in the fuel resistance and an increase in the fuel pellet temperature. However, the amount of the change in fuel pellet temperature is negligible. Changing the fuel pellet radius does not affect the fuel rod temperature profile. The fuel pellet radius increases due to fuel swelling, expansion, and decreases due to fuel densification effects.

Fuel centerline temperature versus fuel pellet radius at different power levels are shown in Figure 3-22. It is seen that fuel centerline temperature and the fuel pellet radius have a linear relationship and with regression coefficient of \( R^2=1 \). At the higher power level, we get a higher fuel centerline temperature.

<table>
<thead>
<tr>
<th>Power Levels (kW/m)</th>
<th>Maximum Fuel Centerline Temperature (°K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.4</td>
<td>1155</td>
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<tr>
<td>33.8</td>
<td>1760</td>
</tr>
<tr>
<td>49.2</td>
<td>2366</td>
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</tbody>
</table>
Table 3-11 Test Points used at Each Power Level

<table>
<thead>
<tr>
<th>Test Number</th>
<th>Fuel Thermal Conductivity (W/m·ºK)</th>
<th>Gap Conductance (W/m²·ºK)</th>
<th>Fuel Pellet Radius (m)</th>
<th>Clad Inside Radius (m)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>2</td>
<td>2.7</td>
<td>4300</td>
<td>0.00609</td>
<td>0.00621</td>
</tr>
<tr>
<td>3</td>
<td>2.7</td>
<td>4300</td>
<td>0.00612</td>
<td>0.00621</td>
</tr>
<tr>
<td>4</td>
<td>2.7</td>
<td>4300</td>
<td>0.00615</td>
<td>0.00621</td>
</tr>
<tr>
<td>5</td>
<td>2.7</td>
<td>4300</td>
<td>0.00618</td>
<td>0.00621</td>
</tr>
<tr>
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<td>4300</td>
<td>0.00621</td>
<td>0.00621</td>
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<td>0.00600</td>
<td>0.00621</td>
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<td>9</td>
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<td>4300</td>
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<td>2.7</td>
<td>4300</td>
<td>0.00591</td>
<td>0.00621</td>
</tr>
</tbody>
</table>

Figure 3-16 Radial Fuel Temperature Profile for a BWR Rod with Changing the Fuel Pellet Radius at $q' = 16.4$ kW/m
Figure 3-17 Radial Temperature Profile for a BWR Rod with Changing the Fuel Pellet Radius at $q' = 32.8 \text{ kW/m}$

Figure 3-18 Radial Temperature Profile for a BWR Rod with Changing the Fuel Pellet Radius at $q' = 49.2 \text{ kW/m}$
**Figure 3-19** Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Fuel Pellet Radius at $q' = 16.4\ kW/m$

**Figure 3-20** Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Fuel Pellet Radius at $q' = 32.8\ kW/m$
Figure 3-21 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Fuel Pellet Radius at $q' = 49.2$ kW/m

Figure 3-22 Fuel Centerline Temperature vs. Fuel Pellet Radius at $q' = 16.4, 32.8, \text{ and } 49.2$ kW/m
3.7 Clad Inside Radius

Effect of clad inside radius on fuel temperature profile was investigated at three different power levels: 16.4, 32.8, and 49.2 kW/m. The total of eleven (11) test points tabulated in Table 3-12 below were calculated at each power level to simulate the effect of the change in the clad inside radius on the fuel rod temperature profile. Figures 3-23, 3-24 and 3-25 show that as the clad inside radius increased keeping the fuel pellet radius constant, the gap thickness between the fuel and the clad is increased and the clad thickness is decreased keeping the clad outside radius constant. There are two mechanisms competing here. One is the increase in the gap thickness, which will cause the fuel temperature to increase and the other is the decrease in the clad thickness. As the clad thickness decreases, the fuel temperature decreases since more heat will be removed from the fuel. The effect of the decrease in the clad thickness is more dominant than the increase in the gap thickness since the clad thermal conductivity is higher than the gap conductance.

The change in the clad inside radius does not change the fuel rod temperature profile. As the clad inside radius increased, the temperature decreased along the fuel radial profile. As the power level increased, the temperature deviation from the reference case is increased. The maximum decrease in deltaT is observed at q’ = 49.2 kW/m and the results are summarized in Table 3-12 below.

<table>
<thead>
<tr>
<th>Power Level q’ (kW/m)</th>
<th>Maximum radial temperature (ºK) deviation from the reference test case Increase (%)</th>
<th>Decrease (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.4</td>
<td>0.4</td>
<td>- 2.5</td>
</tr>
<tr>
<td>32.8</td>
<td>0.6</td>
<td>- 3.3</td>
</tr>
<tr>
<td>49.2</td>
<td>0.6</td>
<td>- 3.7</td>
</tr>
</tbody>
</table>
The clad inside radius is increased due to the fuel expansion, swelling and clad creep down caused by the rod internal pressure and it decreases due to the clad creep down caused by the large primary system pressure relative to the rod internal pressure.

Fuel centerline temperature versus clad inside radius is shown in Figure 3-29 for the three power levels. As the clad inside radius is increased, the fuel centerline temperatures did not see a significant change at each power level. As the power level increased, the fuel centerline temperature increased as seen previously. In conclusion, there is no strong relationship between the clad inside radius and the fuel centerline temperature at a given power level.

**Table 3-13** Test Points used at Each Power Level

<table>
<thead>
<tr>
<th>Test Number</th>
<th>Fuel Thermal Conductivity (W/m·°K)</th>
<th>Gap Conductance (W/m²·°K)</th>
<th>Fuel Pellet Radius (m)</th>
<th>Clad Inside Radius (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00621</td>
</tr>
<tr>
<td>2</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00618</td>
</tr>
<tr>
<td>3</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00615</td>
</tr>
<tr>
<td>4</td>
<td>2.7</td>
<td>4300</td>
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<td>2.7</td>
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<td>2.7</td>
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<td>0.00659</td>
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<tr>
<td>9</td>
<td>2.7</td>
<td>4300</td>
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<td>0.00677</td>
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<tr>
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<td>4300</td>
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<td>0.00696</td>
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<tr>
<td>11</td>
<td>2.7</td>
<td>4300</td>
<td>0.00606</td>
<td>0.00715</td>
</tr>
</tbody>
</table>
Figure 3-23 Radial Temperature Profile for a BWR Rod with Changing Clad Inside Radius at $q' = 16.4 \text{ kW/m}$

Figure 3-24 Radial Temperature Profile for a BWR Rod with Changing Clad Inside Radius at $q' = 32.8 \text{ kW/m}$
Figure 3-25 Radial Temperature Profile for a BWR Rod with Changing Clad Inside Radius at $q' = 49.2$ kW/m

Figure 3-26 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Clad Inside Radius at $q' = 16.4$ kW/m
Figure 3-27 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Clad Inside Radius at $q' = 32.8$ kW/m

Figure 3-28 Radial Temperature Deviation Profile from the BWR Reference Test Case with Changing the Clad Inside Radius at $q' = 49.2$ kW/m
Figure 3-29 Fuel Centerline Temperature vs. Clad Inside Radius at $q' = 16.4$, 32.8, and 49.2 kW/m
3.8 Conclusions

Sensitivity study was performed to investigate the radial fuel rod thermal behavior. Four fuel rod parameters: fuel rod conductivity, gap conductance, fuel pellet radius, and clad inside radius were used and effect of each parameter on the fuel rod radial temperature profile was investigated to understand the model prediction uncertainties. Three power levels 16.4, 32.8, and 49.2 kW/m were used to simulate a typical BWR fuel rod operating condition. The conclusions are summarized as follows:

- The effect of the change in thermal conductivity on the radial temperature profile for a BWR rod was investigated at different power levels. Temperature gradient across the fuel pellet started with a zero gradient at the surface and increased towards the center of the pellet. This concluded that fuel thermal conductivity had a high impact on the fuel centerline temperature compared to the fuel surface. It had no effect on the gap and the clad temperatures. Therefore, it has a high-level impact on the fuel centerline temperature and medium effect on the fuel average temperature.

- The effect of the gap conductance on the fuel rod temperature profile was investigated at three different power levels. It is concluded that temperature deviation due to the change in the gap conductance had a high impact on the fuel pellet temperature and the effect was uniform across the fuel pellet. The deviation in the fuel temperature was the same amount from fuel centerline to surface of the fuel pellet. Therefore, the overall impact on the fuel temperature is high.

- Effect of the fuel pellet radius on the fuel rod temperature profile was investigated at three different power levels. It is concluded that there was not a significant deviation on the fuel temperature due to the change in the fuel pellet radius. Therefore, the overall impact on fuel temperature is low.
Effect of the fuel clad inside radius on the fuel rod temperature profile was investigated at three different power levels. It is concluded that there was a slight deviation on the fuel temperature due to the change in the clad inside radius. Therefore, the overall impact on the fuel temperature is medium. However, the effect on the clad inside temperature is high.

Table 3-14 below summarizes the relationship and the impact matrix for each parameter investigated for the fuel rod temperature profile. This study identifies the critical factors as the fuel thermal conductivity and the gap conductance and also investigated the direct effect of each parameter individually.

However, in real BWR operations, all of these factors are changing simultaneously both in radial and axial directions due to the observed physical mechanisms such as fuel densification, fuel swelling, clad creep down, fuel creep down, fuel clad interaction and the overall process is very complex.

**Table 3-14 Fuel Rod Temperature Profile vs. Fuel Parameters Relationship-Impact Matrix**

<table>
<thead>
<tr>
<th>Fuel temperature</th>
<th>Fuel thermal conductivity $k_f$</th>
<th>Gap conductance $h_g$</th>
<th>Fuel pellet radius $R_f$</th>
<th>Clad inside radius $R_{ci}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel centerline temperature ($T_{\text{max}}$)</td>
<td>H</td>
<td>M</td>
<td>L</td>
<td>L</td>
</tr>
<tr>
<td>Fuel midpoint temperature ($T_{\text{mid}}$)</td>
<td>M</td>
<td>M</td>
<td>L</td>
<td>L</td>
</tr>
<tr>
<td>Fuel surface temperature ($T_{\text{fo}}$)</td>
<td>-</td>
<td>M</td>
<td>L</td>
<td>L</td>
</tr>
<tr>
<td>Fuel average temperature ($T_{\text{avg}}$)</td>
<td>M</td>
<td>M</td>
<td>L</td>
<td>L</td>
</tr>
<tr>
<td>Clad inside temperature ($T_{\text{ci}}$)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>M</td>
</tr>
<tr>
<td>Clad outside temperature ($T_{\text{co}}$)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

*H: High, M:Medium, L:Low*
3.9 References

CHAPTER 4

FUEL THERMAL CONDUCTIVITY MODELS AND SENSITIVITY ANALYSIS

4.1 Introduction

Chapter 4 discusses the model descriptions and comparisons of the three thermal conductivity models: FRAPCON-3.4 Modified NFI Model for UO$_2$ fuels [4, 6], FRAPCON-3.4 Duriez/Modified NFI Model for MOX fuels [4, 6]; and CTF MATPRO-11 Model [1]. Modified NFI model for UO$_2$ fuels and Duriez/Modified NFI model for MOX fuel rods are already compared against MATPRO-11 model and also the experimental data by Luscher et al. in the Material Property Correlations Report [4]. The results from these comparisons are presented in Chapter 4 to demonstrate why modified NFI model for UO$_2$ fuels and Duriez/Modified NFI model for MOX fuels provide the best estimate calculation for the fuel thermal conductivity. CTF MATPRO-11 model is also described and thermal conductivity predictions were compared against the original MATPRO-11 (1979) [1] results between 300°K and 3000°K temperature ranges in Section 4.4. CTF MATPRO-11 model is also compared against MATPRO-11 Rev.2 (1981) [2], MATPRO-11 (1979) [1], Modified NFI model [4], Duriez/Modified NFI model [4], and FRAPCON-3.4 MATPRO-11 [2, 3, 4].

Sensitivity analyses are performed on the modified NFI model by changing the exposure levels and the gadolinium concentrations to create a thermal conductivity database in Section 4.5. Thermal conductivity versus fuel centerline temperatures were plotted to demonstrate the impact of exposure and gadolinium on thermal conductivity. Finally, the modified NFI model predicted fuel thermal conductivity plots that were generated for different exposure levels and gadolinium concentrations were compared against CTF MATPRO-11 model.
4.2 FRAPCON-3.4 Fuel Thermal Conductivity Model Description and Comparisons

FRAPCON-3.4 thermal conductivity model is first originated from MATPRO-11 Rev.2 model [2,3,4] which is a function of temperature, porosity, theoretical density, oxygen-to-metal (O/M) ratio and plutonium content as shown in Equation (4.1).

\[
k = \left( \frac{D}{1+(6.5-0.00469T'(1-D))} \right) \left( \frac{C_v}{(A+BT^{''})(1+3e_{th})} \right) + \ldots \ldots
\]

\[
\ldots 5.2997 \times 10^{-3} T \exp(-\frac{13358}{T}) \left\{ 1+0.169 \left[ \left( \frac{13358}{T} \right) + 2 \right]^2 \right\}
\]  
(Equation 4.1)

Where

\( k \) = thermal conductivity (W/m·°K)

\( D \) = fraction of theoretical density (unitless).

\( C_v \) = phonon contribution to the specific heat at constant volume (J/kg·°K). The first term of the correlation for fuel specific heat capacity is used for this factor.

\( e_{th} \) = linear strain caused by thermal expansion when temperature is >300°K (unitless). The MATPRO correlation for fuel thermal expansion is used for this factor.

\( T \) = fuel temperature (°K).

\( T' \) = porosity correction for temperature,

\( T < 1364°K, T' = 6.50 - T \ (4.69 \times 10^{-3}) \)

\( T > 1834°K, T' = -1 \)

\( 1364°K < T < 1834°K, T' \) is found by interpolation.

\( T^{''} \) = fuel temperature if \( T < 1800°K \)

\( T > 2300°K, T^{''} = 2050°K \)

\( 1800°K < T < 2300°K, T^{''} \) is found by interpolation.
A= a factor proportional to the point defect contribution to the phonon mean free path (m-s/kg°K), the correlation used for this factor is 0.339+12.6 * (absolute value (2.0-O/M ratio).

B= a factor proportional to the phonon-phonon scattering contribution to the phonon mean free path (m-s/kg°K); the correlation used for this factor is 0.06867 * (1+0.6238*plutonium content of the fuel).

The MATPRO-11 model was first used in FRAPCON-2 and then it was updated in the next version of the code, FRAPCON-3, with a thermal conductivity model developed by Lucuta [5,6,7], which accounts for effects of burnup on the thermal conductivity for the irradiated fuels.

Lucuta’s model for fuel thermal conductivity for unirradiated, fully dense urania is presented in Equation 4.2 below:

\[ k_0 = \frac{1}{0.0375+2.165 \times 10^{-4}T} + \left[ \frac{4.715 \times 10^9}{T^2} \right] \exp \left[ -\frac{16361}{T} \right] \]  

(Equation 4.2)

Where

- \( k_0 \): thermal conductivity of unirradiated, fully dense urania (W/m°K)
- \( T \): temperature (°K)

The effect of the dissolved fission products is expressed by a burnup and temperature dependent factor FD in Equation 4.3.

\[ FD = \left[ \frac{1.09}{B^{3.265}} + \frac{0.0643}{\sqrt{B}} \right] \arctan \left[ \frac{1}{\frac{1.99}{B^{2.265}} + \frac{0.0643}{\sqrt{B}}} \right] \]  

(Equation 4.3)

Where,

- \( T \): temperature (°K)
- \( B \): burnup in atom % (1% atom = 9.383 GWd/MTU at 200 MeV/fission)
The effect of the precipitated fission products is expressed by the factor FP in Equation 4.4.

\[ FP = 1 + \left[ \frac{0.019B}{3-0.019B} \right] \left[ \frac{1}{1+\exp\left(\frac{T-1200}{100}\right)} \right] \]  
(Equation 4.4)

The effect of porosity is expressed from Maxwell porosity factor FM in Equation 4.5.

\[ FM = \frac{1-p}{1+(s-1)p} \]  
(Equation 4.5)

where;

P = porosity fraction (as fabricated plus swelling)
S = shape factor (=1.5 for spherical pores)

The radiation effects are given by the factor FR in Equation 4.6.

\[ FR = 1 - \frac{0.2}{1+\exp\left(\frac{T-900}{80}\right)} \]  
(Equation 4.6)

Incorporating all the factors coming from dissolved and precipitated fission gas products, Maxwell porosity effects, radiation effects into the thermal conductivity of irradiated, full dense uranium, thermal conductivity k is given by Equation 4.7.

\[ k = k_0 \times FD \times FP \times FM \times FR \]  
(Equation 4.7)

When Lucuta’s model in FRAPCON-3 was verified against the measured data from Halden Ultra-High Burnup Experiment, it had some drawbacks [4,5,6]. One of the drawbacks was that the model predicted higher temperature values when compared to experimental data temperatures above 2200°K for unirradiated fuel pellets. The other drawback was that it couldn’t predict the effect of burnup degradation on thermal conductivity above ~30 GWd/MTU and thus
had a non-conservative prediction when compared to the high burnup pellet samples. Therefore, a new correlation in the literature was searched to be implemented into FRAPCON-3. Nuclear Fuels Industries (NFI) thermal conductivity model developed by Ohira and Itegaki (1997) [8] was selected and incorporated into FRAPCON-3 to replace the Lucuta’s model [4,5,6,7]. Some modifications were made to the original NFI model for burnup function in the phonon term and also in the electronic term. In addition to that, to capture the effect of the gadolinium addition to the fuel, an adjustment factor which was developed by Massih et al. (1992) [9] was added to the denominator of the phonon term. Since all these modifications are done to the original NFI model, it is called “Modified NFI Model” which incorporates both the burnup and gadolinium effects.

The original NFI model developed by Ohira and Itegaki consists of an electronic contribution term which is inversely proportional to the temperature function $A+BT$ with burnup dependence factors $f(Bu)+g(Bu)h(T)$ in the denominator, plus an electronic term $-CT^2+DT^4$ to account for the radiation effects at high temperatures. The original NFI model which is developed for 95% theoretical density pellet material is shown in Equation 4.8.

$$k_{\text{Original NFI Model}} = \frac{1}{A+BT+f(Bu)+g(Bu)h(T)} \cdot CT^2 + DT^4 \quad \text{(Equation 4.8)}$$

In the modified NFI model, the temperature dependent portion of the burnup function was updated and the form of the electronic term is altered as shown in Equation 4.9 [4,5].

$$k_{\text{Mod. NFI Model}} = \frac{1}{A+a^*gad+BT+f(Bu)+(1-0.9 \exp(-0.04Bu))g(Bu)h(T)} + \frac{E}{T^2} \exp(-\frac{F}{T}) \quad \text{(Equation 4.9)}$$
Where

\( k_{95} \) = Thermal Conductivity for 95\% dense fuel, W/m-°K

\( T \) = Temperature, °K

\( B_u \) = Burnup, GWd/MTU

\( f(B_u) \) = Effect of fission products in crystal matrix (solution) = 0.00187 \* \( B_u \)

\( g(B_u) \) = Effect of irradiation defects

\( = 0.038 \* B_u^{0.28} \)

\( h(T) \) = Temperature dependence of annealing on irradiation defects

\[
h(T) = \frac{1}{1 + 396 \exp \left( \frac{Q}{T} \right)} \quad \text{(Equation 4.10)}
\]

\( Q \) = Temperature dependent parameter = 6380 °K

\( A = 0.0452 \, \text{m-°K/W} \)

\( a = \text{constant} = 1.1599 \)

\( g_{ad} \) = weight fraction of gadolinium

\( B = 2.46 \times 10^{-4} \, \text{m-°K/W/°K} \)

\( E = 3.5 \times 10^9 \, \text{W-°K/m} \)

\( F = 16,361 \, °K \)

The thermal conductivity model is adjusted for as fabricated fuel density using Lucuta’s recommendation for spherical-shaped pores [4,5,6].

\[
k_d = 1.0789 \times k_{95} \times \left( \frac{d}{[1 + 0.5(1-d)]} \right) \quad \text{(Equation 4.11)}
\]
Where

\[ d = \text{density in fraction of TD} \]

\[ k_{95} = \text{as given conductivity based on 95\%TD.} \]

\[ k_d = \text{thermal conductivity adjusted for as fabricated fuel density,} \ d \]

1.0789 is the adjustment factor for conductivity at 100\% TD.

The adjustments to the original NFI model are made on both the phonon term and the electronic term. \((1 - 0.9(\exp(-0.04Bu))\) term is added as a multiplier to the \(g(\text{BU})h(T)\) term in denominator of the phonon term. When compared to the original NFI model, the modification in the phonon term decreases the defect annealing at low burnup; however, it maintains the temperature dependent annealing at higher burnups greater than 40 GWd/MTU such that the phonon term becomes equivalent to the original NFI model. The adjustment in the electronic term was replacing \(-CT^2 + DT^4\) term with \(E/T^2 \exp(-F/T)\) to make it closer to the theoretical based equation from Hagrman et al., and Popov et al. [1,2,3,10]. This modification was shown and mentioned by Ronchi et al. [11] with Institute of Transuranium Elements (ITU) data at on unirradiated PWR pellet material at temperatures approaching fuel melting.

Finally, the modified NFI model is adjusted to account for the gadolinium content from a thermal conductivity correlation developed by Massih et al. [9]. The function of the gad concentration, \(a^*\text{gad}\) term in Massih’s correlation, was incorporated into the modified NFI model in FRAPCON-3.4 as shown in Equation 4.9. The addition of gad concentration to the fuel thermal conductivity correlation is important because nuclear fuel rods include Gadolinia (Gd_2O_3) as burnable absorber to control the power peakings in early life of a fuel assembly. Addition of Gd in UO_2 changes the material properties of the fuel and also the crystal structure of UO_2 and leads to a lower thermal conductivity as a result of phonons scattering with Gad atoms [9].
Model-to-model comparisons of the thermal conductivity values between the modified NFI model and the MATPRO-11 model as a function of temperature are shown by Luscher et al. [4]. Figure 4-1 demonstrates the comparisons of the two models and shows that the thermal conductivities predicted by the MATPRO-11 model are lower than the thermal conductivities predicted by the modified NFI model across the applicable temperature range (i.e., 500°K to 300°K) for unirradiated UO₂. The reason for this difference is that the modified NFI model has the exposure effect in the thermal conductivity calculations and accounts for the degradation of fuel thermal conductivity with increasing burnup [4]. On the other hand, the MATPRO-11 model does not account for the exposure effect in the thermal conductivity calculations. Figure 4-1 also demonstrates the decrease in the thermal conductivity using the modified NFI model with burnup level of 30 GWd/MTU. It is seen clearly from Figure 4-1 that the thermal conductivity degrades with increasing burnup. The decrease in the thermal conductivity with increasing burnup continues up to around 2000°K where phonon term is dominant and then the thermal conductivity starts to slightly increase above 2000°K where radiation effects start.

Model-to-experimental data comparisons for MATPRO-11 and the modified NFI model for both unirradiated and irradiated UO₂ are shown by Luscher et al. and documented in the Material Property Correlations report [4]. Figure 4-2 shows the comparisons of the experimental data to the predicted data from MATPRO-11 model for unirradiated UO₂. It is seen from Figure 4-2 that MATPRO-11 model under predicts some of the data for the thermal conductivity of unirradiated UO₂. The average bias and standard deviation in the predictions were 9.5% and 11% respectively [4]. Figure 4-3 shows the comparisons of the measured data to predicted data from the modified NFI model. It is seen from Figure 4-3 that the modified NFI model also underpredicts some of the data the data like MATPRO-11 model. However, the modified NFI model had a smaller bias 2.4% and a smaller standard deviation 8%. It is concluded that the
smaller bias and standard deviation show that the modified NFI model better estimates the thermal conductivities than the MATPRO-11 model.

Model-to-measured data comparisons of MATPRO-11 and the modified NFI model for irradiated UO\textsubscript{2} were demonstrated by Luscher et al [4]. Comparison of the results revealed that MATPRO-11 overpredicts the thermal conductivities when compared to the experimental data as it is seen in Figure 4-4. The bias was reported as 40% with a standard deviation of 31% [1]. On the other hand, the modified NFI model predicted the experimental data very well as shown in Figure 4-5. Only a small amount of data was overpredicted with 5% bias and 8% standard deviation. Figure 4-4 and Figure 4-5 show clearly that the modified NFI model predicts thermal conductivities for irradiated UO\textsubscript{2} much better than the MATPRO-11 model since it accounts for the degradation of thermal conductivity with increasing burnup.

\begin{figure}[h]
\centering
\includegraphics[width=0.7\textwidth]{Figure_4-2.png}
\caption{MATPRO-11 and Modified NFI Thermal Conductivity Models for UO\textsubscript{2} as a Function of Temperature. [4]}
\end{figure}
Figure 4-3 MATPRO-11 Model to Data Comparison for Thermal Conductivity of Unirradiated UO$_2$[4]

Figure 4-4 Modified NFI Model to Data Comparison for Thermal Conductivity of Unirradiated UO$_2$[4]
Figure 4-5 MATPRO-11 Model to Data Comparison for Thermal Conductivity of Irradiated UO$_2$ [4]

Figure 4-6 Modified NFI Model to Data Comparison for Thermal Conductivity of Irradiated UO$_2$ [4]
Duriez/modified NFI model for MOX fuels already exists in FRAPCON-3.4. The model is developed by combining the Duriez stoichiometry-dependent correlation and modified NFI model [4,13]. Duriez correlation is derived from diffusivity measurements on unirradiated fuel pellets and modified NFI model included the burnup degradation effects. The Duriez thermal conductivity correlation has greater dependence of MOX, but only a minor dependence on plutonium content [4].

The Duriez/modified NFI model is given by:

\[
k_{95} = \frac{1}{A(x) + a \cdot \text{gad} + B(x)T + f(Bu) + (1 - 0.9 \exp(-0.4Bu))g(Bu)h(T) + C_{\text{mod}}\frac{T^2}{T}} \exp\left(-\frac{D}{T}\right)
\]

(Equation 4.12)

where:

\(k_{95}\) = Conductivity at 95% theoretical density, W/m·°K

\(x\) = 2.00-O/M

\(T\): Temperature, °K.

\(A(x) = 2.85x + 0.035\), m·°K/W

\(B(x) = (2.86 - 7.15x) \times 10^{-4}\) m/W

\(C = 1.689 \times 10^9\), W·°K/m

\(D = 13520\) °K

\(A = 1.1599\)

\(\text{Gad}\) = Weight fraction gadolinium

\(\text{Bu}\) = Burnup in GWd/THM

\(f(Bu)\) = Effect of fission products in crystal matrix (solution), 0.00187 \(\times\) Bu

\(g(Bu)\) = Effect of irradiated defects, 0.038\(\times\)Bu\(^{0.28}\)

\(h(T)\) = Temperature dependence of annealing on irradiated defects, \(\frac{1}{1 + 396\exp\left(-\frac{Q}{T}\right)}\)
\[ Q = \text{Temperature dependent parameter} = 6380 \, ^\circ\text{K} \]

\[ C_{\text{mod}} = 1.5 \times 10^9 \, \text{W}^{-\circ}\text{K}/\text{m} \]

Model-to-model comparisons of the thermal conductivity values between Duriez/modified NFI model and the MATPRO-11 model for MOX fuel as a function of temperature is demonstrated by Luscher et al. [4]. Figure 4-6 gives the comparisons of the two models and shows that the thermal conductivities predicted by the MATPRO-11 model are lower than the thermal conductivities predicted by Duriez/modified NFI model across the applicable temperature range (i.e., 500°K to 300°K) for MOX fuel. Figure 4-6 also demonstrates that there is a decrease in the thermal conductivity when Duriez/modified NFI model is used with burnup level of 30 GWd/MTU. It is seen clearly from Figure 4-6 that thermal conductivity degrades with increasing burnup.

**Figure 4-6** MATPRO-11 and Duriez/Modified NFI Thermal Conductivity Models for MOX as a Function of Temperature. [4]
Model-to-measured data comparisons of MATPRO-11 and the Duriez/modified NFI model for unirradiated MOX are demonstrated by Luscher et al. and documented in the Material Property Correlations report [4]. Comparison of the results shows that MATPRO-11 underpredicts the thermal conductivities when compared to the experimental data as it is seen in Figure 4-7. The average bias in the MATPRO-11 predictions is reported as 9% with 6% standard deviation for both 3 and 15 wt% plutonium concentrations [4]. On the other hand, Duriez/modified NFI model predicts experimental data very well as shown in Figure 4-8. The average bias in Duriez/modified NFI model is reported to be less than 2% with a standard deviation less than 3%. Figure 4-8 demonstrates that Duriez/modified NFI model predicts better than MATPRO-11 model for MOX fuels with a smaller bias and standard deviation.

Figure 4-7 MATPRO-11 Model to Data Comparison for Thermal Conductivity of MOX Fuel [4]
Conclusions from the comparisons from the thermal conductivity models is that modified NFI model for UO$_2$ fuels and Duriez/modified NFI model for MOX fuels are the best estimate thermal conductivity models in the literature which takes in to account the degradation of fuel thermal conductivity with high burnup and effects of gadolinium concentration.
4.3 Application Ranges of Modified NFI Model and Duriez/Modified NFI Model

Application ranges for the modified NFI model and Duriez/Modified NFI model to calculate the thermal conductivity of UO\(_2\) and MOX is as follows [4]:

- Temperature: 300°K to 3000°K
- Rod average burnup: 0 to 62 GWd/MTU
- As-fabricated density: 92 to 97 percent theoretical density
- Gadolinia content: 0 to 10 wt%.

It is recommended that the modified NFI model and Duriez/modified NFI model should be used within these applicable ranges to get the best estimates of the UO\(_2\) and MOX thermal conductivity.

4.4 CTF Fuel Thermal Conductivity Model

CTF [12] currently uses MATPRO-11 fuel thermal conductivity model from 1979 which depends on only temperature [1]. Equation 4.13 below shows that the MATPRO-11 model does not account for the exposure dependence and the gadolinia concentration. MATPRO-11 model in CTF is used for both UO\(_2\) and MOX fuel rods.

The thermal conductivity \(k_{UO_2}\) in MATPRO-11 is calculated from Equation 4.13 below:

\[
k_{UO_2} = \left[ \max \left( 0.0191 \frac{40.4}{(T-273.15)+464} + 1.216 \times 10^{-4} e^{(1.867 \times 10^{-3} \times (T-273.15))} \right) \right] C \quad \text{(Equation 4.13)}
\]

Where

\(k_{UO_2} = \text{Fuel thermal conductivity, W/m·°K}\)

\[C = 100 \times \left[ \frac{1 - \beta (1-f_D)}{1-0.05\beta} \right] \quad \text{(Equation 4.14)}\]

\[\beta = 2.58 - (5.8 \times 10^{-4}) (T-273.15) \quad \text{(Equation 4.15)}\]

\(T\) : Temperature, °K
Both current MATPRO 11 model in CTF shown in Equation 4.13 and MATPRO-11 model from NUREG/CR-0497 (1979) \[1\] were solved analytically at 95% theoretical density and the thermal conductivities were compared for validation purposes. Comparisons of the results are demonstrated in Figure 4-9. It is seen clearly from Figure 4-9 that both of the MATPRO correlations predict the same thermal conductivity. As temperature increases from 300°K to 2000°K, the thermal conductivity decreases showing the phonon contributions and after 2000°K thermal conductivity starts to increase due to the electronic contributions.

The thermal conductivity ranges from 8 to 2 W/m-K as the fuel temperature changes from 300°K to 3000°K. This analysis will be used later to compare the CTF MATPRO-11 model to FRAPCON-3.4 modified NFI model over the BWR and PWR steady state operating temperatures in order to investigate the effect of the exposure and the gadolinium on the fuel thermal conductivity.

Figure 4-10 shows the comparison of the thermal conductivity models between MATPRO-11 from 1979, CTF MATPRO-11, FRAPCON-3.4 MATPRO-11 Rev.2 and modified NFI model across the applicable temperature range. It is seen from Figure 4-10 that CTF currently has MATPRO-11 model from 1979. When the CTF MATPRO-11 model is compared against the modified NFI model at 0 GWD/MTU, it is observed that both models give the same thermal conductivity values up to 2000°K. Above 2000°K, CTF starts to overpredict the thermal conductivities. On the other hand, MATPRO-11 Rev.2 model always underpredicts the thermal conductivities when compared to the modified NFI model.
Figure 4-9 Comparison of Fuel Thermal Conductivities between CTF and MATPRO-11

Figure 4-10 Comparison of Fuel Thermal Conductivity Models between CTF, MATPRO-11, and the Modified NFI
Figure 4-11 shows the comparison of the thermal conductivity models between MATPRO-11 from 1979, CTF MATPRO-11, FRAPCON-3.4 MATPRO-11 Rev.2 and Duriez/modified NFI model across the applicable temperature range. It is seen from Figure 4-11 that CTF currently has the original MATPRO-11 model from 1979. When the CTF MATPRO-11 model is compared against the Duriz/modified NFI model at 0 GWD/MTU, it is observed that CTF MATPRO-11 model overpredicts the thermal conductivities since it doesn’t take into account the stoichiometry and MOX fuel thermal conductivity is strongly influenced by the oxygen to metal ratio.
4.5 Sensitivity Analysis on FRAPCON-3.4 Fuel Thermal Conductivity Model and Database

FRAPCON-3.4 fuel thermal conductivity model described in Section 4.1 was solved numerically. Sensitivity analyses were performed to study the impact of the gadolinium concentration and the exposure on the fuel thermal conductivity of UO₂ fuel. The main goal was to create a thermal conductivity database for a typical BWR and PWR operating conditions. The results of this study will help us understand the impact of the increased exposure and the gadolinium concentration on the fuel thermal conductivity and also give us information on the expected operating conductivity ranges.

FRAPCON-3.4 has the modified NFI model which accounts for the degradation of the fuel thermal conductivity with increasing burnup and gadolinium concentration. The modified NFI model was solved numerically at burnup levels of 0, 30 and 60 GWd/MTU and the gadolinium concentration was increased from 0 Gd w/o to 10 Gd w/o incrementally as shown in Figure 4-12 through Figure 4-15.

Figure 4-12 shows the impact of increasing gadolinium concentration on the fuel thermal conductivity. Gad concentration is increased from 0 Gd w/o to 10 Gd w/o for unirradiated UO₂ fuel across the applicable temperature range (from 300°K to 3000°K). It is seen from Figure 4-12 that as the Gad concentration increases, the fuel thermal conductivity degrades gradually up to 2000°K. The thermal conductivity values drop from around 8 W/m-°K to 4 W/m-°K. The minimum is observed at 2000°K as 2 W/m-K. The amount of the variation in thermal conductivity between the highest (10 Gd w/o) and the lowest gadolinium concentration decreases as temperature increases from 300°K to 2000°K. Above 2000°K, all the curves show the recovery phase in thermal conductivity indicating an increase in thermal conductivity from 2 W/m-°K to 3
The other observation is that the thermal conductivity curves follow similar trend, showing a negligible gadolinium effect above 2000°K.

**Figure 4-12** Modified NFI Model Thermal Conductivity as a Function of Temperature with Increasing Gadolinium Concentration (at 0 GWd/MTU)

Figure 4-13 shows the impact of increasing gadolinium concentration on the fuel thermal conductivity at exposure level of 30 GWd/MTU. The same type of trend is observed in Figure 4-13 as it is seen in Figure 4-12. As Gad concentration is increased, the fuel thermal conductivity degrades gradually from 4 W/m·°K to 2.7 W/m·°K. As temperature increases from 300°K to 2000°K, the change in fuel thermal conductivity decreases. After 2000°K, all the curves show the same trend showing negligible gadolinium effect. The minimum thermal conductivity 1.6 W/m·°K is observed around 2000°K. Above 2000°K, due to the electronic contributions, the thermal conductivity increases from 1.6 W/m·°K to 2.7 W/m·°K.
Figure 4-14 shows the impact of increasing gadolinium concentration on the fuel thermal conductivity at the exposure level 60 GWd/MTU. The same type of trend is observed in Figure 4-14 as it is seen in Figure 4-12 and Figure 4-13. As Gad concentration is increased, the fuel thermal conductivity degrades gradually from 3 W/m°K to 2.2 W/m°K. As temperature increases from 300°K to 2000°K, the change in fuel thermal conductivity decreases. Above 2000°K, all the curves show the same trend showing a negligible gadolinium effect. The minimum thermal conductivity 1.5 W/m°K is observed around 2000°K. Above 2000°K, due to the electronic contributions, the thermal conductivity increases from 1.5 W/m°K to 2.7 W/m°K.
Figure 4-14 Modified NFI Model Thermal Conductivity as a Function of Temperature with Increasing Gadolinium Concentration (at 60 GWd/MTU)

Figure 4-15 shows the exposure effect on the thermal conductivity predicted by FRAPCON-3.4 modified NFI model for 0 w/o Gd case. As burnup increases, the fuel thermal conductivity decreases between the temperatures 300°K to 2000°K. Above 2000°K, all the curves show the same trend regardless of the exposure.
4.6 Comparisons of CTF versus FRAPCON-3.4 Thermal Conductivity Sensitivity Analysis

The CTF MATPRO-11 fuel thermal conductivity model described in Section 4.3 was solved numerically to perform sensitivity analysis to see the impact of the exposure and the gadolinium on the fuel thermal conductivity. Thermal conductivity results obtained from the CTF MATPRO-11 model were compared against the results obtained from the FRAPCON-3.4 modified NFI model described in Section 4.2.

Figure 4-16 shows the comparison of the fuel thermal conductivities predicted by CTF and FRAPCON-3.4 as a function of temperature for different exposure levels with 0 w/o Gd concentration. It is seen from Figure 4-16 that the CTF MATPRO-11 model and the modified NFI model predict almost the same fuel thermal conductivities at 0 exposure and 0 w/o Gd case between 300°K and around 2000°K. However, CTF starts to overpredict the thermal conductivities above 2000°K where radiation effects start. As the exposure increases, the thermal
conductivities predicted by the modified NFI model decreases. CTF overpredicts the thermal conductivities for all the exposed cases since it doesn’t take into account the burnup effects.

Figure 4-17 shows the comparison of the fuel thermal conductivities predicted by CTF and FRAPCON-3.4 as a function of temperature for different Gd concentrations at 0 exposure level. It is seen from Figure 4-17 that the CTF MATPRO-11 model and the modified NFI model predict almost the same fuel thermal conductivities at 0 exposure and 0 w/o Gd case between 300°K and around 2000°K. However, CTF starts to overpredict the thermal conductivities above 2000°K where radiation effects start. As the Gd concentration increases, the thermal conductivities predicted by the modified NFI model decreases gradually. CTF overpredicts the thermal conductivities for all the Gd cases since it doesn’t take into account the Gadolinium concentration.

Figure 4-18 shows the comparison of fuel thermal conductivities predicted by CTF and FRAPCON-3.4 as a function of temperature for different Gd concentrations at 30 GWd/MTU exposure level. It is seen from Figure 4-18 that the CTF MATPRO-11 model overpredicts the fuel thermal conductivities for all the cases since it cannot capture the burnup effects.

Figure 4-19 shows the comparison of the fuel thermal conductivities predicted by CTF and FRAPCON-3.4 as a function of temperature for different Gd concentrations at 60 GWd/MTU exposure level. It is seen from Figure 4-19 that CTF with MATPRO-11 overpredicts the fuel thermal conductivities for all the cases since it cannot capture the burnup effects.
Figure 4-16 Effect of Exposure on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model

Figure 4-17 Effect of Gadolinium Concentration on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model (at 0 GWd/MTU)
**Figure 4-18** Effect of Gadolinium Concentration on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model (at 30 GWd/MTU)

**Figure 4-19** Effect of Gadolinium Concentration on Fuel Thermal Conductivity vs. Temperature for FRAPCON-3.4 Modified NFI and CTF MATPRO-11 Model (at 60 GWd/MTU)
4.7 References


CHAPTER 5

CTF AND FRAPCON-3.4 BENCHMARK STUDIES ON FUEL THERMAL CONDUCTIVITY PREDICTIONS

The modified NFI fuel thermal conductivity model was successfully implemented in CTF. A new input called IFRAP is created to invoke the new model as an option. In order to keep backwards compatibility, CTF MATPRO-11 model is kept available to the users. When IFRAP=1, CTF will use the modified NFI model and when IFRAP=0, CTF will use the MATPRO-11 model.

Chapter 5 summarizes the benchmark studies on fuel thermal conductivity between CTF and FRAPCON-3.4. CTF predicted thermal conductivity values were compared against the FRAPCON-3.4 predictions to validate the CTF updated model results.

Section 5.1 describes the comparisons of the fuel thermal conductivities between the current CTF with MATPRO-11 model and the updated CTF with the modified NFI model. One example test case was selected from FRAPTRAN 1.4 Integral Assessment as benchmark cases [1]. Section 5.1 shows the thermal conductivity comparison analysis performed for a PWR fuel rod, REP- Na3, CABRI reactor test case from FRAPTRAN 1.4 Integral Assessment [1].

5.1 Numerical Comparisons of Fuel Thermal Conductivity Predictions between CTF MATPRO-11 Model and CTF Modified NFI Model

The fuel thermal conductivities as calculated with the CTF MATPRO-11 model and the CTF modified NFI model were compared. REP-Na3 and FK1 FRAPCON-3 base irradiation cases from FRAPTRAN 1.4 Integral Assessment were selected to simulate a PWR fuel rod.
Section 5.1 describes the thermal conductivity comparisons performed for a PWR single fuel rod, REP-Na3, with the current CTF with MATPRO-11 and the improved CTF with the modified NFI model.

Single channel, single center PWR fuel rod was modeled with CTF. The modified NFI model is integrated into CTF as a new option invoked by the new defined input IFRAP. When IFRAP= 1, CTF uses the modified NFI model and when IFRAP= 0, it uses the current MATPRO-11 thermal conductivity model. Steady-state thermal conductivities were retrieved from both cases and tabulated as a function of temperature.

CTF MATPRO-11 thermal conductivity model does not account for the degradation of fuel thermal conductivity with increasing burnup. On the other hand, the modified NFI model accounts for the exposure and the gadolinium content change.

Figure 5-1 shows the comparisons of the thermal conductivities predicted by the current MATPRO-11 model and the modified NFI model integrated into CTF. IFRAP= 1 option which uses the modified NFI model is run with 0 w/o Gd and 0 GWD/MTU exposure. The comparison of the two models shows that both of the models predict the almost same thermal conductivities at 0 GWD/MTU exposure and 0 w/o Gd.
The same example PWR rod was selected to demonstrate that the new model in CTF can show the degradation of thermal conductivity with Gd concentration and burnup. Figure 5-2 demonstrates that the CTF MATPRO-11 model predicts almost the same thermal conductivity values at 0 GWd/MTU exposure and 0 w/o Gd concentration, but due to the lack of burnup and Gd dependence it cannot capture the thermal conductivity degradation.
Figures 5-3 and 5-4 show the comparison of the FRAPCON-3.4 and CTF predicted thermal conductivities at different exposure and gadolinium concentrations. FRAPCON-3.4 modified NFI model is solved numerically across the correlation temperature range between 300°K to 3000°K. CTF steady-state thermal conductivity predictions for a typical PWR fuel rod is in the range of 600°K to 900°K as shown in Figure 5-3 and 5-4. It is confirmed from these figures that the modified NFI model implemented in CTF works properly and predicts the correct thermal conductivities.
Figure 5-3 Comparisons of CTF predicted Fuel Thermal Conductivities vs. Fuel Temperature for Single Center PWR at Different Gd Concentration and 0 GWd/MTU

Figure 5-4 Comparisons of CTF predicted Fuel Thermal Conductivities to FRAPCON-3.4 Predictions for PWR Rod at Different Gd Concentration and 30 GWd/MTU
5.2 References

CHAPTER 6

CTF AND FRAPCON-3.4 BENCHMARK STUDIES
ON FUEL CENTERLINE TEMPERATURE

Chapter 6 summarizes the benchmark studies on fuel centerline temperatures between Halden reactor test assembly data [1,2,3,4]; FRAPCON-3.4 [4,5,6]; and CTF [7] predictions.

Five test cases are selected from FRAPCON Integral Assessment for comparisons to Halden Reactor experiments: (1) During first ramp to power (BOL, UO₂); (2) throughout life (burnup, UO₂); (3) Burnup with 2% Gd₂O₃; (4) Burnup with 8% Gd₂O₃; and (5) MOX case with burnup. Fuel centerline temperature predictions from the current and updated fuel thermal conductivity model in CTF are compared against the Halden experimental test data and FRAPCON-3.4 predictions. The reason why these rods are selected for comparison to experimental data is that they are representatives for all different conditions including BOL and burnup conditions as well as different Gd concentrations and different fuel rods, UO₂ and MOX rods. In addition to that the rods selected for comparison are solid rods so that a good comparison can be made for the fuel centerline temperatures.

Section 6.1 describes the benchmark studies on the fuel centerline temperatures predicted by CTF against the Halden reactor test assembly experimental data experimental data and FRAPCON-3.4 predictions for IFA-432 rod 1 UO₂ at BOL conditions.

Section 6.2 describes the benchmark studies on the fuel centerline temperatures predicted by CTF against the Halden reactor test assembly experimental data experimental data and FRAPCON-3.4 predictions for IFA-432 rod 1 UO₂ with burnup of 45 GWD/MTU.

Section 6.3 describes the benchmark studies on the fuel centerline temperatures predicted by CTF against the Halden reactor test assembly experimental data experimental data and FRAPCON-3.4 predictions for IFA-681 rod 2 UO₂+2%Gd₂O₃ with burnup of 23 GWD/MTU.
Section 6.4 describes the benchmark studies on the fuel centerline temperatures predicted by CTF against the Halden reactor test assembly experimental data and FRAPCON-3.4 predictions for IFA-681 rod 3 UO₂ + 8%Gd₂O₃ with burnup of 57 GWD/MTU.

Section 6.5 describes the benchmark studies on the fuel centerline temperatures predicted by CTF against the Halden reactor test assembly experimental data and FRAPCON-3.4 predictions for IFA-610 rod 2 MOX fuel rod with burnup of 58 GWD/MTU.

Section 6.6 summarizes the all data statistics to demonstrate statistically how the new burnup dependent fuel thermal conductivity model implemented in CTF predicts the fuel centerline temperatures. Descriptive Statistics were performed to analyze the mean and standard deviation of the predicted fuel centerline temperature for all cases.

6.1 Assessment of Fuel Centerline Temperature Predictions at BOL

The BOL fuel centerline temperature predictions are compared against the measurements taken during first ramp to power for IFA-432r1 from Halden experiments [1]. First ramp to power takes place during the first 1 or 2 days of operation. Since this is a short time period, initial fuel rod dimensions will still be valid because there will be no time to change in dimensions due to fission gas release, fuel densification, swelling, cladding creeps, or corrosion [1]. There will be only thermal expansion due to temperature increase.

IFA-432r1 is selected from FRAPCON-3.4 Integral Assessment study for comparison of the fuel centerline temperatures. Fuel centerline temperatures predicted by CTF are compared against FRAPCON-3.4 predictions and the experimental data. Figure 6.1 shows the comparison of fuel centerline temperature predicted by CTF with IFRAP=0 (current model); CTF with IFRAP=1 (updated model); FRAPCON-3.4; and the measured data for IFA-432r1 at BOL. It is seen from Figure 6-1 that both CTF and FRAPCON-3.4 give excellent predictions which are within 5% error band. Current MATPRO-11 model in CTF (IFRAP=0) also predicts the fuel centerline temperature at BOL as good as CTF with the updated model
(IFRAP=1) and FRAPCON-3.4. Both of the codes predict the fuel centerline temperature within 5% error band.

![Predicted vs. Measured Fuel Centerline Temperature](image)

**Figure 6-1** IFA-432r1 BOL UO₂ Fuel Centerline Temperature Predictions

### 6.2 Assessment of Fuel Centerline Temperature Predictions for Burnup Case

The assessment of fuel centerline temperature predictions by CTF is performed using IFA-432r1 exposed UO₂ with burnup of 45 GWD/MTU from Halden reactor test assemblies [1] to evaluate CTF’s ability to account for the fuel thermal conductivity degradation with burnup. Figure 6-2 shows the linear heat generation rate (LHGR) as a function of burnup. LHGR is around 12 kW/ft (3.66 kW/m) at the beginning of life and then starts to decrease to 9.2 kW/ft (2.80 kW/m) on average. Figure 6-3 shows fuel centerline temperature profile versus rod average burnup for the measured data, FRAPCON-3.4, CTF with IFRAP=1 and IFRAP=0 predictions. It is seen from Figure 6-3 that CTF with IFRAP=1 option gives good agreement with both the data and FRAPCON-3.4 predictions and has 0.9848 mean and 0.0157 standard deviation. On the other hand, CTF with IFRAP=0 option predicts the data well at first time step, around 0 GWD/MTU and then as burnup increases, it starts to underpredict the temperature and deviates
from the measured data. The reason for the underprediction in fuel centerline temperature with IFRAP=0 option is that MATPRO-11 model in CTF does not take into account the thermal conductivity degradation with increasing burnup resulting in higher thermal conductivity and lower temperature predictions.

Figure 6-4 shows predicted vs. measured fuel centerline temperature for IFA-432 rod 1. It is seen from Figure 6-4 that CTF with IFRAP=1 predicted fuel centerline temperatures are within 5% error band and agrees well with the experimental data. On the other hand, CTF with IFRAP=0 option underpredicts the fuel centerline temperatures and predicted fuel centerline temperatures are outside the 5% error band.

Figure 6-5 shows predicted minus measured divided by measured fuel centerline temperature vs. rod average burnup for FRAPCON-3.4 and CTF with IFRAP=1 predictions. It is seen from Figure 6-5 that CTF with IFRAP=1 predicts within 5% error band.

![Figure 6-2 IFA-432r1 UO₂ LHGR vs. Fuel Rod Average Burnup](image)
Figure 6-3 Fuel Centerline Temperature vs. Rod Average Burnup for IFA-432r1

Figure 6-4 Predicted vs. Measured Fuel Centerline Temperature for IFA-432r1 UO₂ at 45 GWD/MTU
6.3 Assessment of Temperature Predictions for UO₂ + 2%Gd₂O₃ Fuel Rod

The assessment of fuel centerline temperature predictions by CTF is performed using IFA-681 rod 2 UO₂ + 2%Gd₂O₃ fuel rod from Halden reactor test assemblies [2] to evaluate CTF’s ability to account for the fuel thermal conductivity degradation with burnup and gadolinium concentration.

IFA-681r2 is selected for comparison of the analysis because it is a solid rod and has 2 % Gd which consists of standard Gd (contains ¹⁵⁵Gd or ¹⁵⁷Gd). This allows investigating the degradation of fuel thermal conductivity due to Gd and also the effect of neutron absorption by Gd atoms on the radial power profile.

Figure 6-6 shows the linear heat generation rate versus rod average burnup. It is seen from Figure 6-6 that during first rise to power, linear heat generation rate goes around 11 kW/ft (3.35 kW/m) and after that point it shows oscillations between 9 kW/ft and 11 kW/ft.
Figure 6-7 shows the comparison of fuel centerline temperature predicted by FRAPCON-3.4, CTF with IFRAP=1 and IFRAP=0 options against the measured data as a function of rod average burnup. It is seen from Figure 6-7 that both CTF and FRAPCON-3.4 underpredicts the data during first rise to power until 5 GWD/MTU. The reason for the underprediction in this region is that there is uncertainty in the measured rod power as Gd burns out. After all the Gd burns out the effect of Gd on the rod power decreases and only affect would be on the thermal conductivity. After 5 GWD/MTU, both FRAPCON-3.4 and CTF with IFRAP=1 give good agreement with the experimental data. CTF with IFRAP=1 option gives good agreement with the data with 1.002 mean and 4.5 % standard deviation.

Figure 6-8 shows predicted vs. measured fuel centerline temperature for IFA-681r2. It is seen from Figure 6-8 that CTF with IFRAP=1 gives excellent predictions and gives almost the same temperature values with FRAPCON-3.4. On the other hand CTF IFRAP=0 underpredicts the fuel centerline temperature since it doesn’t take into account the burnup and Gd effects on fuel thermal conductivity.

Figure 6-9 shows predicted minus measured divided by measured data vs. rod average burnup. It is shown in Figure 6-10 that CTF with IFRAP=1 predicted fuel centerline temperatures are within 10% error band.
Figure 6-6 Linear Heat generation Rate vs. Rod Average Burnup for IFA-681r2 UO$_2$+2\%Gd$_2$O$_3$

Figure 6-7 Fuel Centerline Temperatures vs. Rod Average Burnup for IFA-681r2 UO$_2$+2\%Gd$_2$O$_3$
Figure 6-8 Predicted vs. Measured Fuel Centerline Temperature for IFA-681r2 UO$_2$+2%Gd$_2$O$_3$

Figure 6-9 Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-681r2
6.4 Assessment of Temperature Predictions for UO₂+ 8%Gd₂O₃ Fuel Rod

This section summarizes the assessment of fuel centerline temperature predictions for IFA-681 rod 3 with UO₂+8%Gd₂O₃ fuel rod from Halden reactor test assemblies [2]. Rod 3 is selected for comparisons because it is a solid rod and has 8% Gd concentration which is higher than Rod 2 described in section 6.3 and also it contains standard Gd (contains ⁵⁵Gd or ⁵⁷Gd). CTF’s ability to account for the fuel thermal conductivity degradation with burnup and gadolinium concentration is investigated.

It is shown in FRAPCON-3.4 Integral Assessment [4] that FRAPCON-3.4 predictions shows excellent agreement when it is compared to experimental data until 200 days and after 200 days FRAPCON-3.4 overpredicts the temperatures by up to 100ºK and the reason for this overprediction is not clear. It is stated in FRAPCON-3.4 Integral Assessment on page A.39 that “For rod 3, there are some overpredictions (50 to 120 C) in the third and fourth cycles. This may be due to error in the temperature measurement or the estimation of the rod power level. This seems likely because the power level during these cycles is reported to increase from about 21 kW/m to about 25 kW/m, while temperature is reported to remain constant at about 850C. It also seems strange for the power level in this rod to increase during these cycles while the power level in the other rods is constant during these cycles”.

Since there are some uncertainties in the reported temperature data, CTF temperature prediction comparisons and statistical calculations are performed until 200 days. After 200 days, a couple of test points are run with CTF to demonstrate that CTF also overpredicts after 200 days and predictions are in line with FRAPCON-3.4.

Figure 6-10 shows the linear heat generation rate versus rod average burnup. It is seen from Figure 6-10 that during first rise to power, linear heat generation rate goes up to around 7 kW/ft (2.13 kW/m) and after that point it shows some oscillations between 7 kW/ft and 8 kW/ft (2.44 kW/m).

Figure 6-11 shows the comparison of fuel centerline temperature predicted by FRAPCON-3.4, CTF with IFRAP=1 and IFRAP=0 option against the measured data as a function of rod average burnup.
It is seen from Figure 6-11 that CTF with IFRAP=1 option gives good agreement with the data with 0.983 mean and 3.5% standard deviation.

Figure 6-12 shows predicted minus measured divided by measured data vs. rod average burnup. It is shown in Figure 6-12 that CTF with IFRAP=1 predicted fuel centerline temperatures are within 10% error band.

Figure 6-13 shows predicted vs. measured fuel centerline temperature for IFA-681r3. It is seen from Figure 6-13 that CTF with IFRAP=1 option gives excellent predictions and gives almost the same temperature values with FRAPCON-3.4. On the other hand CTF IFRAP=0 underpredicts the fuel centerline temperature.

Figure 6-10 Linear Heat generation Rate vs. Rod Average Burnup for IFA-681r3 UO₂+8%Gd₂O₃
Figure 6-11 Fuel Centerline Temperatures vs. Rod Average Burnup for IFA-681r3 UO$_2$+8%Gd$_2$O$_3$

Figure 6-12 Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-681r3
6.5 Assessment of Fuel Centerline Temperature for MOX Fuel Rod

The assessment of fuel centerline temperature predictions by CTF for MOX fuel rod is performed using IFA-610 rod 2 from Halden reactor test assemblies [3]. Fuel centerline predictions from CTF with IFRAP=1 is compared against the predictions from CTF with IFRAP=0, FRAPCON-3.4 and experimental data.

IFA-610 rod 2 is base irradiated for four cycles in the French Gravelines-4 reactors to burnup level of 55 MWD/kgM and then it is refabricated and instrumented with a centerline thermocouple to be used for cladding liftoff experiments in Halden reactor [1, 3].

Figure 6-14 shows the linear heat generation rate versus rod average burnup starting from the fresh fuel. The period rod stayed in Halden reactor starts from burnup level of 54 GWD/MTU. The
LHGRs used from Figure 6-14 for the fuel centerline temperature comparisons are between burnup levels of approximately 54 GWD/MTU to 57 GWD/MTU.

Figure 6-15 shows fuel centerline temperature predicted by CTF IFRAP=1; IFRAP=0; FRAPCON-3.4; and the experimental data as function of data measurement time. It is seen from Figure 6-15 that CTF with IFRAP=1 shows good agreement with the data; whereas CTF with IFRAP=0 underpredicts the temperatures 200 °K lower at all the times.

Figure 6-16 shows predicted vs. measured fuel centerline temperature for IFA-610 rod 2. It is seen from Figure 6-16 that CTF with IFRAP=1 predicted fuel centerline temperatures are within 5% error band and agrees well with the experimental data. On the other hand, CTF with IFRAP=0 option underpredicts the fuel centerline temperatures and predicted fuel centerline temperatures are outside the 5% error band.

Figure 6-17 shows predicted minus measured divided by measured fuel centerline temperature vs. rod average burnup for FRAPCON-3.4 and CTF with IFRAP=1 predictions. It is seen from Figure 6-17 that CTF with IFRAP=1 predicts within 5% error band.

![Figure 6-14 Linear Heat generation Rate vs. Rod Average Burnup for IFA-610r2 MOX Fuel Rod](image-url)
Figure 6-15 Fuel Centerline Temperatures vs. Rod Average Burnup for IFA-610r2 MOX Fuel Rod

Figure 6-16 Predicted vs. Measured Fuel Centerline Temperature for IFA-610r2 MOX Fuel Rod
Figure 6-17 Predicted minus Measured divided by Measured Fuel Centerline Temperature vs. Rod Average Burnup for IFA-610r2

6.6 Statistical Analysis of CTF Fuel Centerline Temperature Predictions

All data points used in CTF predictions are combined together to see the overall picture. Predicted versus measured fuel centerline temperatures, normalized fuel centerline temperatures versus rod average burnup and descriptive statistics analysis are performed and shown in Figure 6-19 and 6-23.

Figure 6-18 shows comparison of the predicted fuel centerline temperature against the measured data for all data points. It is shown from Figure 6-18 that CTF with IFRAP=1 predictions are within 5% error band and shows a linear profile for all the five cases.

Figure 6-19 shows normalized fuel centerline temperature versus rod average burnup for all data points predicted by CTF using IFRAP=1 option.

Table 6-1 summarizes the mean and standard deviation of each case analyzed.
In summary, CTF with IFRAP=1 option predictions are performed using fifty-eight (58) data points and have a mean of 1.0082 and a standard deviation of 0.0382. On the other hand, FRAPCON-3.4 predictions are performed using one hundred and twenty-eight (128) data points and have a mean of 1.0038 and a standard deviation of 0.0340. When statistical analysis are performed for FRAPCON-3.4 using the same data cases as CTF (58 data points), mean becomes 0.9981 and standard deviation decreases to 0.0329.

Figure 6-20, 6-21 and 6-22 show the descriptive statistics for all normalized fuel centerline temperature data predicted from CTF with IFRAP=0, IFRAP=1 and FRAPCON-3.4, respectively.
Figure 6-19 Normalized Fuel Centerline Temperature vs. Rod Average Burnup for IFA-432r1 BOL, IFA-432r1 burnup, IFA-681r2 UO₂+2%Gd₂O₃, IFA-681r3 UO₂+8%Gd₂O₃, and IFA-610r2 MOX
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Figure 6-20 Descriptive Statistics for CTF with IFRAP=0 Normalized Fuel Centerline Temperature

Descriptive Statistics

Variable: CTF IFRAP=0

Anderson-Darling Normality Test
A-Squared: 3.107
P-Value: 0.000

Mean: 0.892024
StDev: 0.062005
Variance: 4.93E-03
Skewness: 1.91E+10
Kurtosis: -1.5E-01
N: 58

Minimum: 0.78770
1st Quartile: 0.84030
Median: 0.87390
3rd Quartile: 0.92510
Maximum: 1.96580

95% Confidence Interval for Mu
0.87300 to 0.91024

95% Confidence Interval for Sigma
0.05588 to 0.08484

95% Confidence Interval for Median
0.84008 to 0.88447

Descriptive Statistics

Variable: CTF IFRAP=1

Anderson-Darling Normality Test
A-Squared: 0.671
P-Value: 0.076

Mean: 1.00818
StDev: 0.03817
Variance: 1.46E-03
Skewness: -2.2E-02
Kurtosis: -8.1E-01
N: 58

Minimum: 0.92230
1st Quartile: 0.96153
Median: 1.00670
3rd Quartile: 1.04715
Maximum: 1.08310

95% Confidence Interval for Mu
0.99915 to 1.01622

95% Confidence Interval for Sigma
0.03227 to 0.04674

95% Confidence Interval for Median
0.99634 to 1.02777

Figure 6-21 Descriptive Statistics for CTF with IFRAP=1 Normalized Fuel Centerline Temperature
Descriptive Statistics

Variable: FRAPCON-3.4

- Anderson-Darling Normality Test
  - A-Squared: 0.028
  - P-Value: 0.717
- Mean: 1.0005
- Std Dev: 0.0304
- Variance: 1.56E-03
- Skewness: 1.48E-02
- Kurtosis: 0.199622
- N: 128
- Minimum: 0.92500
- 1st Quartile: 0.98500
- Median: 1.0015
- 3rd Quartile: 1.0225
- Maximum: 1.10900

- 95% Confidence Interval for μ:
  - Lower: 0.99750
  - Upper: 1.00979

- 95% Confidence Interval for σ:
  - Lower: 0.0032
  - Upper: 0.03981

- 95% Confidence Interval for Median:
  - Lower: 1.00070
  - Upper: 1.00846

Figure 6-22 Descriptive Statistics for FRAPCON-3.4 Normalized Fuel Centerline Temperature
6.7 References


CHAPTER 7

SINGLE AND MULTI CHANNEL STEADY STATE CALCULATIONS USING
COUPLED NEUTRONICS/THERMAL HYDRAULICS/ FUEL PERFORMANCE
CODE

Chapter 7 summarizes code-to-code comparisons between CTF/TORT-TD and CTF/TORT-TD/FRAPTRAN coupled codes for fuel temperature predictions.

CTF/TORT-TD coupled code calculations are performed using two models: 1) The current MATPRO-11 fuel thermal conductivity model (option IFRAP=0); and 2) The new improved fuel thermal conductivity model (option IFRAP=1).

In the coupled code CTF/TORT-TD/FRAPTRAN, the fuel rod is modeled with FRAPTRAN by bypassing the CTF fuel rod model. Single and multi-channel steady state cases are run with both of the coupled codes and fuel centerline and surface temperatures are compared. Note that when CTF/TORT-TD/FRAPTRAN coupled code is run at steady state conditions, it switches to FRAPCON calculation and when transient cases are run it switches to FRAPTRAN calculation. Although in this chapter the coupled code is called CTF/TORT-TD/FRAPTRAN, it uses FRAPCON for steady-state calculations.

Section 7.1 summarizes the fuel temperature comparisons between the two coupled codes for single fuel rod at steady state conditions. Section 7.1.1 shows results for UO₂ high burnup; section 7.1.2 shows results for MOX high burnup single fuel rod centered in a single channel configuration. Temperature predictions from CTF/TORT-TD with IFRAP=0 and IFRAP=1 options are compared against CTF/TORT-TD/FRAPTRAN fuel temperature predictions.

Section 7.2 summarizes the fuel temperature comparisons between the two coupled codes for a Purdue benchmark case [1], 4x4 PWR bundle, multi-channel steady state conditions. Section 7.2.1 shows steady state fuel temperature comparisons between CTF/TORT-TD/FRAPTRAN and CTF/TORT-TD, in which CTF uses a constant gap conductance; and Section 7.2.2 shows steady state fuel temperature
comparisons between CTF/TORT-TD/FRAPTRAN and CTF/TORT-TD, in which CTF uses its dynamic gap conductance model.

### 7.1 Single Channel Fuel Temperature Comparisons

Two set of problems, one for high burnup UO₂ rod and one for high burnup MOX fuel rod, are designed using single fuel rod centered in a single channel configuration shown as in Figure 7-1. The purpose of this design is to test CTF/TORT-TD/FRAPTRAN and CTF/TORT-TD coupled codes for one single channel configuration and also to investigate the differences between the fuel rod models in CTF and FRAPTRAN. Testing of single fuel rod within a single channel configuration will clearly show the comparisons between the two fuel rod models in CTF, with IFRAP=0 and with IFRAP=1 against FRAPTRAN since the configuration will only focus on one rod and eliminate the effects of surrounding rods to the sub-channels if a multi-channel configuration were used.

![Single fuel rod centered in a single channel](image)

**Figure 7-1** Single fuel rod centered in a single channel

Section 7.1.1 shows the results for UO₂ single fuel rod; and section 7.1.2 shows the results for MOX single fuel rod. Both of the fuel rods have 35 GWD/MTU burnup and the simulations are carried out at steady-state Hot Full Power (HFP) conditions. The HFP case is used to test the effect of different spatial distributions of power and fuel temperature; and to evaluate how it is affected by the two fuel rod models.
The geometry and the composition of each fuel pin are obtained from the Purdue MOX benchmark which is a 4x4 arrangement and will be discussed in Section 7.2. One high burnup UO2 and one high burnup MOX fuel rod are selected for the simulation of the test cases presented in this section.

The UO2 fuel pin consists of 4.25% enriched Uranium Oxide from an assembly with an average enrichment of 4.2 %; and the MOX fuel pin consists of 5.0 % Plutonium Oxide from an assembly with an average 4.3 % PuO2. [2]

The fuel rod and nuclear model descriptions for each code are provided in Section 7.2.

7.1.1 UO2 Single Channel Fuel Temperature Comparisons

The UO2 single fuel rod centered in a single channel configuration is simulated with both CTF/TORT-TD/FRAPTRAN and CTF/TORT-TD coupled codes. CTF/TORT-TD is executed using the two fuel thermal conductivity models - the current MATPRO-11 model IFRAP=0 and the new burnup dependent fuel thermal conductivity model IFRAP=1. Fuel centerline and fuel surface temperatures are compared between the following three models:

1) CTF/TORT-TD with IFRAP=0 – the fuel pin is modeled by CTF without burnup dependent fuel conductivity;

2) CTF/TORT-TD with IFRAP=1 – the fuel pin is modeled by CTF with burnup dependent fuel conductivity;

3) CTF/TORT-TD /FRAPTRAN – the fuel pin is modeled by FRAPTRAN with burnup dependent fuel conductivity.

In this section, CTF/TORT-TD results obtained using an axially constant gap conductance are presented. An axially constant gap conductance is used to simplify the model and to reduce the computational time.
Figure 7-2 shows the fuel centerline temperature versus fuel axial height for the three models. It is seen from Figure 7-2 that CTF with the IFRAP=0 option underpredicts the fuel centerline temperature, whereas CTF with the IFRAP=1 option shows a significant improvement on fuel centerline temperature predictions and matches well with the FRAPTRAN predictions. CTF with the IFRAP=0 option underpredicts the fuel centerline temperature when compared to FRAPTRAN predictions, because it doesn’t take into account the burnup dependence of the fuel thermal conductivity, which results in predicting a higher heat transfer across the fuel pin and therefore in lower temperatures.

Figure 7-3 shows CTF versus FRAPTRAN predicted fuel centerline temperatures. It is seen from Figure 7-3 that there is an average of 200ºK difference between the IFRAP=0 and IFRAP=1 options.

Fuel pellet surface temperatures predicted with the three models are also compared and shown in Figure 7-4. The axially constant gap conductance model used in CTF and the axially varying gap conductance model used in FRAPTRAN are shown in Figure 7-5. Figure 7-4 shows that FRAPTRAN gives an average of 10ºK higher prediction in pellet surface temperature, since it has much lower gap conductance than CTF above 2m of the fuel height as shown in Figure 7-5.

The radial and axial power profiles used in all three models are provided in Figure 7-6 and Figure 7-7.
Figure 7-2 Fuel Centerline Temperature vs. Axial Position for UO$_2$ High Burnup Fuel Rod

Figure 7-3 CTF vs. FRAPTRAN Fuel Centerline Temperature
Figure 7-4 Fuel Pellet Surface Temperature vs. Axial Position for UO₂ High Burnup Fuel Rod

Figure 7-5 Gap Conductance vs. Axial Position for UO₂ High Burnup Fuel Rod
Figure 7-6 Relative Power vs. Normalized Fuel Pellet Radius

Figure 7-7 Axial Power Profile
7.1.2 MOX Single Channel Fuel Temperature Comparisons

The calculations performed in section 7.1.1 are repeated for a MOX fuel rod to test the performance of the new fuel thermal conductivity model for MOX fuel. The CTF/TORT-TD coupled code is used with the IFRAP=0 and IFRAP=1 option.

Figure 7-8 shows the fuel centerline temperature vs. fuel axial height as predicted with the three models. It is seen from Figure 7-8 that CTF with the IFRAP=0 option underpredicts the fuel centerline temperature, whereas CTF with the IFRAP=1 option shows a significant improvement in the fuel centerline temperature predictions and agrees well with the FRAPTRAN predictions. As discussed previously, CTF with the IFRAP=0 option underpredicts the temperature, because it doesn’t take into account the fuel thermal conductivity degradation with burnup.

Figure 7-9 compares the fuel centerline temperatures as predicted with the two CTF options, IFRAP=0 and IFRAP=1. It is seen from Figure 7-9 that above 1400ºK, the deviation between the two models increases and becomes more than 200ºK.

The fuel pellet surface temperatures are also compared between the three models and shown in Figure 7-10. The axially constant gap conductance model used in CTF and the axially varying gap conductance model used in FRAPTRAN are shown in Figure 7-11. Figure 7-10 indicates that FRAPTRAN has less than 10ºK higher prediction in fuel pellet surface temperature since it has much lower gap conductance than CTF above 2m of the fuel height (see Figure 7-11). This difference occurs due to the difference in the gap conductance in the upper part of the fuel rod (above 2m).

The radial power profile used in all three models is provided in Figure 7-12; and the axial power profile is the same as used for UO₂ fuel rod (given in Figure 7-7).
Figure 7-8 Fuel Centerline Temperature vs. Axial Position for MOX High Burnup Fuel Rod

Figure 7-9 CTF vs. FRAPTRAN Fuel Centerline Temperature
Figure 7-10 Fuel Pellet Surface Temperature vs. Axial Position for MOX High Burnup Fuel Rod

Figure 7-11 Gap Conductance vs. Axial Position for MOX High Burnup Fuel Rod
The conclusions from the single fuel rod steady state calculations are as follows:

1) CTF/TORT-TD with IFRAP=1 option gives consistent results with CTF/TORT-TD/FRAPTRAN code for steady state single fuel rod configuration demonstrating that CTF with the new fuel thermal conductivity model can model the fuel rod as well as FRAPTRAN; therefore, CTF/TORT-TD with IFRAP=1 calculations can be carried out instead of CTF/TORT-TD/FRAPTRAN calculation to save computational time and simplify the process.

2) CTF/TORT-TD with IFRAP=0 option underpredicts fuel centerline temperature relative to CTF with IFRAP=1 and FRAPTRAN predictions as expected since MATPRO-11 fuel thermal conductivity model does not take into account burnup degradation effects.

Figure 7-12 Radial Power Profile vs. Normalized Fuel Pellet Radius
3) The use of an axially constant gap conductance does not have a significant effect on the fuel centerline temperature. It only affects the fuel pellet surface temperature within 10ºK differences for the two fuel rods analyzed in this section.

### 7.2 Multi-Channel Fuel Temperature Comparisons

In this section, a 4x4 PWR fuel bundle configuration from the Purdue MOX benchmark [1], as shown in Figure 7-13, is used to assess the new thermal conductivity model fuel temperature predictions for multi-rod/ multi-channel configuration. The configuration consists of 15 PWR pins and one control rod guide tube in a 4x4 array. There are 4 fuel rod groups in 15 PWR pins: low burnup MOX, high burnup MOX, low burnup UO$_2$ and high burnup UO$_2$. In addition to that, this system will allow testing the two fuel rod models in CTF and FRAPTRAN for different fuel types with different burnup levels [2].

![Figure 7-13 4x4 PWR Pin Array and Subchannel Configuration [2]](image)

HFP steady state calculations are performed using CTF/TORT-TD with the IFRAP=0 and IFRAP=1 options, where the fuel rod is modeled with CTF. The same test case is simulated with
CTF/TORT-TD/FRAPTRAN, where the fuel rods are modeled with FRAPTRAN and the calculated fuel temperatures are compared. FRAPCON is used to initialize the fuel conditions for FRAPTRAN calculations. HFP conditions are used to simulate more realistic reactor environment, where the spatial distributions of power and fuel temperature are of significant importance.

### 7.2.1 Description of the Models Utilized in the Codes

The geometry and the composition of each fuel rod are obtained from the Purdue MOX benchmark [1]. Cross-sections needed for TORT-TD calculations are taken from a previous research study [2]. The models developed for each code are described in Sections 7.2.1.1 through 7.2.1.4.

The cold, as-manufactured, fuel dimensions are given in Table 7-1. The same dimensions are used within the two coupled code systems.

<table>
<thead>
<tr>
<th>As-manufactured cold fuel dimensions [2]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active Length [m]</td>
</tr>
<tr>
<td>Pin pitch [m]</td>
</tr>
<tr>
<td>Fuel pellet radius [m]</td>
</tr>
<tr>
<td>Inner clad radius [m]</td>
</tr>
<tr>
<td>Outer clad radius [m]</td>
</tr>
<tr>
<td>Clad-pellet gap thickness [m]</td>
</tr>
<tr>
<td>Clad thickness [m]</td>
</tr>
</tbody>
</table>

### 7.2.1.1 Description of the FRAPCON Model

One MOX and one UO₂ fuel rod models are prepared for FRAPCON calculations. The Purdue benchmark data does not include certain geometry information such as the plenum length and pellet dish size, which is required as an input for FRAPCON; therefore these values are set to the values obtained from sample input decks [2].

Both fuel rod types were burned for a total of 1000 days at a constant, axially-uniform power, which was calculated as the average-pin nominal power from the benchmark.
Table 7-2 summarizes the input parameters used in FRAPCON for both of the fuel types. Table 7-3 shows the nodalization parameters and Table 7-4 shows the fuel parameters for each fuel type.

**Table 7-2** Input parameters for both of the fuel types [2]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cold plenum length [m]</td>
<td>0.22</td>
</tr>
<tr>
<td>Outer diameter of plenum spring [m]</td>
<td>0.007902</td>
</tr>
<tr>
<td>Diameter of the plenum spring wire [m]</td>
<td>0.001006</td>
</tr>
<tr>
<td>Number of turns in the plenum spring</td>
<td>20</td>
</tr>
<tr>
<td>Length of each pellet [m]</td>
<td>0.011003</td>
</tr>
<tr>
<td>Depth of pellet dish [m]</td>
<td>0.000280</td>
</tr>
<tr>
<td>Pellet dish shoulder width [m]</td>
<td>0.001036</td>
</tr>
<tr>
<td>Pellet surface roughness [m]</td>
<td>2.10^{-6}</td>
</tr>
<tr>
<td>Expected density increase during operation [kg/m³]</td>
<td>100.</td>
</tr>
<tr>
<td>Clad type</td>
<td>Zircaloy 4</td>
</tr>
<tr>
<td>Cladding inner surface roughness [m]</td>
<td>5.0038 10^{-7}</td>
</tr>
<tr>
<td>Initial gas pressure [Pa]</td>
<td>2.0 10^6</td>
</tr>
<tr>
<td>Coolant pressure [MPa]</td>
<td>15.5</td>
</tr>
<tr>
<td>Coolant inlet temperature [°K]</td>
<td>560</td>
</tr>
<tr>
<td>Coolant mass flux [kg/(m² s)]</td>
<td>3062.88</td>
</tr>
<tr>
<td>Linear power [kW/m] (axially uniform)</td>
<td>19.13</td>
</tr>
<tr>
<td>Time step interval size [days]</td>
<td>50</td>
</tr>
<tr>
<td>Burn time [days]</td>
<td>1000</td>
</tr>
</tbody>
</table>

**Table 7-3** Nodalization of FRAPCON models for both of the fuel types [2]

<table>
<thead>
<tr>
<th>Nodalization Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet radial nodes (equal cross-sectional area)</td>
<td>17</td>
</tr>
<tr>
<td>Axial nodes (equal length)</td>
<td>20</td>
</tr>
</tbody>
</table>

**Table 7-4** Fuel parameters for each fuel type [2]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-235 enrichment [%]</td>
<td>4.25</td>
</tr>
<tr>
<td>PuO₂ content [%]</td>
<td>N/A</td>
</tr>
<tr>
<td>% of theoretical density</td>
<td>93.35</td>
</tr>
</tbody>
</table>

**7.2.1.2 Descriptions of the FRAPTRAN Model**

FRAPTRAN gets most of the data from FRAPCON restart file. FRAPCON restart file will be different depending on the fuel type and the burn time at which the fuel properties are obtained. Table 7-5 shows the FRAPTRAN input parameters used for all rods. Table 7-6 shows FRAPTRAN
initialization times for each fuel type at different burnup levels and Table 7-7 shows radial and axial nodalization inputs.

**Table 7-5** FRAPTRAN input parameters for all rods [2]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper plenum volume [m$^3$]</td>
<td>1.1114 x 10$^{-5}$</td>
</tr>
<tr>
<td>Number of coils in upper plenum spring</td>
<td>5</td>
</tr>
<tr>
<td>Uncompressed height of upper plenum spring [m]</td>
<td>0.0281</td>
</tr>
<tr>
<td>Uncompressed outer diameter of upper plenum spring [m]</td>
<td>0.007902</td>
</tr>
<tr>
<td>Diameter of upper plenum spring wire [m]</td>
<td>0.0010</td>
</tr>
<tr>
<td>Pellet dish depth [m]</td>
<td>0.00104</td>
</tr>
<tr>
<td>Pellet dish volume [m$^3$]</td>
<td>2.06 x 10$^{-7}$</td>
</tr>
<tr>
<td>As-fabricated fill gas temperature [ºK]</td>
<td>295.15</td>
</tr>
</tbody>
</table>

**Table 7-6** FRAPCON initialization time for each fuel rod type [2]

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>FRAPCON Initialization Time [seconds]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Low Burnup (0.15 MWD/kg)</td>
</tr>
<tr>
<td>UO$_2$</td>
<td>299883.</td>
</tr>
<tr>
<td>MOX</td>
<td>304887.</td>
</tr>
</tbody>
</table>

**Table 7-7** Nodalization inputs for FRAPTRAN [2]

<table>
<thead>
<tr>
<th>Nodalization Input</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellet radial nodes (equal cross-sectional area)</td>
<td>15</td>
</tr>
<tr>
<td>Cladding radial nodes</td>
<td>2</td>
</tr>
<tr>
<td>Axial nodes (equal length)</td>
<td>20</td>
</tr>
</tbody>
</table>

**7.2.1.3 Description of the CTF Model**

The CTF model, as shown in Figure 7-13, consists of 15 fuel rods and one control guide tube, all arranged in a 4x4 array of 25 sub-channels. There are three sub-channel geometries consisting of central, side, and corner, and two sub-channel transvers-connection geometries consisting of half and full gap width. Sub-channel geometry values used in the CTF input decks are provided in Table 7-8 and sub-channel transverse connection geometry values are provided in Table 7-9. Modeling options are selected based on the recommended and/or typical values for a PWR, and are provided in Table 7-10. Boundary conditions for coolant enthalpy, mass flow and outlet pressure are obtained from the Purdue benchmark data, with the flow rate based on the average flow over 4 pins and given in Table 7-11. Table 7-12 shows
the radial and axial nodalization and Table 7-13 gives the spacer grid information used in CTF calculations [2].

### Table 7-8 Sub-channel geometry type information [2]

<table>
<thead>
<tr>
<th>Sub-channel type</th>
<th>Area [m$^2$]</th>
<th>Wetted Perimeter [m]</th>
<th>Number of Sub-channels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central</td>
<td>0.0000928</td>
<td>0.0288</td>
<td>9</td>
</tr>
<tr>
<td>Side</td>
<td>0.0000464</td>
<td>0.0144</td>
<td>12</td>
</tr>
<tr>
<td>Corner</td>
<td>0.0000232</td>
<td>0.00720</td>
<td>4</td>
</tr>
</tbody>
</table>

### Table 7-9 Sub-channel horizontal connection type information [2]

<table>
<thead>
<tr>
<th>Sub-channel connection type</th>
<th>Length [m]</th>
<th>Width [m]</th>
<th>Horizontal Loss Coefficient</th>
<th>Number of Gaps</th>
</tr>
</thead>
<tbody>
<tr>
<td>Half gap width</td>
<td>0.0126</td>
<td>0.001717</td>
<td>0.5</td>
<td>16</td>
</tr>
<tr>
<td>Full gap width</td>
<td>0.0126</td>
<td>0.003434</td>
<td>0.5</td>
<td>24</td>
</tr>
</tbody>
</table>

### Table 7-10 Modeling options used in CTF [2]

<table>
<thead>
<tr>
<th>Modeling option</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rod friction model</td>
<td>$\lambda = 0.204Re^{-0.2}$</td>
</tr>
<tr>
<td>Entrainment/deposition</td>
<td>Original model</td>
</tr>
<tr>
<td>Mixing / void drift</td>
<td>Specify mixing coefficient</td>
</tr>
<tr>
<td>Equilibrium drift factor</td>
<td>1.4</td>
</tr>
<tr>
<td>2-phase turbulent mixing coefficient</td>
<td>0.004</td>
</tr>
<tr>
<td>Maximum time step size [s]</td>
<td>0.01 for steady state 0.001 during rod ejection</td>
</tr>
</tbody>
</table>

### Table 7-11 CTF boundary conditions [2]

<table>
<thead>
<tr>
<th>Boundary condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet enthalpy [kW/kg]</td>
<td>1267.9</td>
</tr>
<tr>
<td>Inlet mass flow [kg/s]</td>
<td>4.5465</td>
</tr>
<tr>
<td>Outlet pressure [MPa]</td>
<td>15.5</td>
</tr>
</tbody>
</table>
Table 7-12 CTF radial and axial nodalization [2]

<table>
<thead>
<tr>
<th>Pellet radial nodes (equal mesh)</th>
<th>15</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cladding radial nodes</td>
<td>2</td>
</tr>
<tr>
<td>Axial nodes (equal length)</td>
<td>20</td>
</tr>
</tbody>
</table>

Table 7-13 CTF spacer grid information [2]

<table>
<thead>
<tr>
<th>Spacer grid loss coefficient</th>
<th>1.701</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of spacer grids</td>
<td>10 (at even-numbered nodes)</td>
</tr>
</tbody>
</table>

CTF fuel rod model uses the dimensions shown in Table 7-1 with fresh UO$_2$ standard MATPRO-11 fuel properties for both UO$_2$ and MOX fuel rods. Fuel properties used in CTF are provided in Table 7-15.

CTF uses two fuel rod models in its calculations:

1) The IFRAP=0 option uses the current MATPRO-11 fuel thermal conductivity, which is a function of temperature for both UO$_2$ and MOX fuel rods. It also uses the UO$_2$ fuel properties for MOX fuel rods.

2) The IFRAP=1 option uses the modified NFI fuel thermal conductivity model, for the UO$_2$ fuel rods and the modified Duriez /NFI fuel thermal conductivity model for the MOX fuel rods.

Both of these models are used first with a constant gap conductance and then with a dynamic gap conductance model. There will be total of 4 scenarios, as shown in Table 7-14, for the steady state multi-channel analysis.

Table 7-14 CTF fuel rod models

<table>
<thead>
<tr>
<th>Fuel Rod Models</th>
<th>Fuel Thermal Conductivity Model</th>
<th>Gap Conductance</th>
</tr>
</thead>
<tbody>
<tr>
<td>IFRAP=0</td>
<td>MATPRO-11</td>
<td>Constant</td>
</tr>
<tr>
<td>IFRAP=1</td>
<td>Modified/NFI for UO$_2$ or Duriez/NFI for MOX</td>
<td>Constant</td>
</tr>
</tbody>
</table>
### Table 7-15 CTF fuel properties [2]

<table>
<thead>
<tr>
<th>Fuel properties</th>
<th>Built-in UO₂ properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clad properties</td>
<td>Build-in zirconium-dioxide properties</td>
</tr>
<tr>
<td>% Theoretical fuel density</td>
<td>93.35</td>
</tr>
</tbody>
</table>

#### 7.2.1.4 Description of the TORT-TD Model

TORT-TD performs three-dimensional (3D) steady-state/transient neutron-kinetics calculations. TORT-TD model uses 8 neutron energy groups and S₈ angular discretization with symmetric, equal angular mesh sizes.

TORT-TD model shown in Figure 7-14 has 16 nodes on the x-y plane – one for each fuel rod or guide tube. It has 40 axial nodes in the active core region. In addition, a reflector region is modeled above and below the active core [2].

### Table 7-16 TORT-TD model properties [2]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of energy groups</td>
<td>8</td>
</tr>
<tr>
<td>Number of delayed neutron precursors</td>
<td>6</td>
</tr>
<tr>
<td>Legendre scattering order</td>
<td>1</td>
</tr>
<tr>
<td>Quadrature type</td>
<td>Symmetric</td>
</tr>
<tr>
<td>Quadrature order</td>
<td>S₈</td>
</tr>
</tbody>
</table>

### Table 7-17 TORT-TD axial nodalization [2]

<table>
<thead>
<tr>
<th>Region</th>
<th>Length [m]</th>
<th>Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active core</td>
<td>3.6576</td>
<td>40 (equal size)</td>
</tr>
<tr>
<td>Lower reflector</td>
<td>0.3</td>
<td>5 (equal size)</td>
</tr>
<tr>
<td>Upper reflector</td>
<td>0.3</td>
<td>5 (equal size)</td>
</tr>
</tbody>
</table>

TORT-TD assembly arrangement is shown in Figure 7-14 and the corresponding fuel rod and sub-channel arrangement for CTF is shown in Figure 7-13. It is seen from Figure 7-14 that XY plane is divided into four regions and each region has four fuel pins. Four regions consists of low burnup MOX,
high burnup MOX, low burnup UO\textsubscript{2} and high burnup UO\textsubscript{2}. Low burnup UO\textsubscript{2} region has one control rod guide tube with three UO\textsubscript{2} pins [2].

![Figure 7-14 TORT-TD Assembly Arrangement [2]](image)

The cross section libraries used are generated by HELIOS [2] and Table 7-18 shows the names of the cross-sections libraries used for each fuel pin. Note that each region (UO\textsubscript{2}, MOX, control guide tube and reflector) is modeled separately.

The power input to TORT-TD, shown in Table 7-19, is determined by the pin-average nominal power for 15 fuel pins for the HFP steady state case. The Hot Zero Power (HZP) at the beginning of the Rod Ejection Accident (REA) is taken as 0.01% of this value [2].

For the HFP steady state, the control rod is fully withdrawn. However, in the rod ejection accident, the rod begins inserted to 50% of the length of the core, and is withdrawn at a constant rate between 1.0 and 1.1 seconds, as shown in Figure 7-15.
Figure 7-15 Control Rod Insertion during Rod Ejection Accident [2]

Table 7-18 Cross-section libraries [2]

<table>
<thead>
<tr>
<th>Region</th>
<th>Cross section library name</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO2 pin</td>
<td>WQ-U42-FF-unrodded, WQ-U42-FF-rodded</td>
</tr>
<tr>
<td>Control rod guide tube</td>
<td>WQ-U42-GT-unrodded, WQ-U42-GT-rodded</td>
</tr>
<tr>
<td>MOX pin</td>
<td>WQ-M43-HF-unrodded</td>
</tr>
<tr>
<td>Reflector</td>
<td>WQ-U42-RF-unrodded</td>
</tr>
</tbody>
</table>

Table 7-19 Initial steady-state power [2]

<table>
<thead>
<tr>
<th>Power (HFP) [MW]</th>
<th>1.04952</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power (HZP) [MW]</td>
<td>1.04952 \times 10^{-4}</td>
</tr>
</tbody>
</table>

7.2.2 Steady State Fuel Temperature Comparisons

Four cases starting at HFP steady state conditions are calculated with CTF/TORT-TD:

1) CTF with the IFRAP=0 option - the current MATPRO-11 fuel thermal conductivity model and a constant gap conductance;
2) CTF with the IFRAP=1 option - the new fuel thermal conductivity model and a constant gap conductance;

3) CTF with the IFRAP=0 option - the current MATPRO-11 fuel thermal conductivity model and the dynamic gap conductance model of CTF;

4) CTF with the IFRAP=1 option - the new fuel thermal conductivity model and the dynamic gap conductance model of CTF.

The fuel temperature predictions from the four cases are compared against the CTF/TORT-TD/FRAPTRAN predictions, in which the fuel rod is modeled with the FRAPTRAN fuel thermal conductivity and gap conductance models. The purpose of these comparisons is to investigate the impact of using new fuel thermal conductivity model in CTF on fuel centerline predictions and also demonstrate the effect of axially varying gap conductance on fuel centerline predictions.

7.2.2.1 Steady State Fuel Temperature Comparisons using a Constant Gap Conductance

This section summarizes the fuel temperature predictions by CTF/TORT-TD with IFRAP=0 and IFRAP=1 options; and using an axially constant gap conductance. Comparisons are provided for the fuel temperature predictions of the two models in CTF to the FRAPTRAN predictions for the configuration shown in Figure 7-13. One fuel rod from each rod type is selected to demonstrate the comparison results. Figure 7-16 through Figure 7-24 show the comparisons of the fuel temperature predictions for rod 6, 7, 10 and 11, respectively.

Figure 7-16 shows temperature comparisons for rod 6 which is a low burnup MOX rod. CTF uses the IFRAP=0 option for the predictions in Figure 7-16, which consists of four sub-figures. From left to right it has, gap conductance, fuel temperature (which includes, center, surface and average fuel temperature), fuel temperature drop and clad/coolant temperature drop comparisons. It is seen from gap conductance plot that CTF uses a constant gap conductance, whereas FRAPTRAN uses an axially varying gap conductance where gap conductivity is calculated internally. The FRAPTRAN gap conductance has a
peak in the middle part of the fuel rod where the power has a maximum. The fuel center, average and surface temperature comparisons show that CTF underpredicts the fuel centerline temperature as compared to FRAPTRAN and the difference increases toward the upper part of the fuel rod. This underprediction is combination of two effects: the differences in the fuel thermal conductivity model; and the differences in the gap conductance model. The fuel surface temperature predicted by FRAPTRAN is higher in the regions where the gap conductance is lower and lower in the regions where it is higher, as expected. Although there is a significant difference in the gap conductance values used in both of the codes, as shown in Figure 7-16 the impact on the fuel surface temperature is less than 40ºK.

The temperature drop in the gap and across the fuel pellet shows that FRAPTRAN predicts around 100ºK higher temperature drop since CTF predicts lower temperatures than FRAPTRAN. The temperature drop in the clad and clad surface shows that both codes have the same clad and coolant properties, the same heat transfer coefficient and clad conductivity, predicting the same temperature drop in the clad and clad surface.

Figure 7-17 shows the same type of calculations performed by CTF using the IFRAP=1 option. The improvement in the fuel centerline temperature is observed clearly. Using the IFRAP=1 option in CTF increases the predicted temperatures leading to better agreement with the FRAPTRAN predictions. There are some points which are slightly different and the difference is occurring due to the difference in gap conductance values used in the two codes.

Figures 7-18 and 7-19 show the temperature comparisons for Rod 7, which is a high burnup MOX fuel rod. Figure 7-18 shows the comparisons for CTF with the IFRAP=0 option. It is seen from the gap conductance plot that in the middle part of the fuel rod, where the power is highest, both of the codes use the same gap conductance. In Figure 7-18, a significant difference between the CTF and the FRAPTRAN fuel temperature predictions are observed. The differences seen in the FRAPTRAN and the CTF temperature predictions are due to the difference in the fuel thermal conductivity models of the two codes. CTF with the IFRAP=0 option uses MATPRO-11 model, whereas FRAPTRAN uses the
Duriez/Modified NFI fuel thermal conductivity model. It is seen from fuel temperature predictions comparisons that CTF always predicts lower fuel centerline and fuel average temperatures compared to FRAPTRAN when IFRAP=0 option is used. The fuel pellet surface temperature predictions of the codes are exactly the same since both codes use the same gap conductance values in the middle section of the rod, where the power is the highest. It is demonstrated that the difference in the gap conductance values in the upper and lower fuel rod parts, where the power is lowest, do not play a significant role in the fuel pellet surface temperature predictions. Figure 7-19 shows fuel temperature predictions by CTF using the IFRAP=1 option, which utilizes the Duriez/Modified NFI model for MOX fuel rods. It is seen from Figure 7-19 that using the IFRAP=1 option in CTF clearly improves the predictions and agrees well with the FRAPTRAN predictions.
Figure 7-16 CTF with IFRAP= 0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6 (Low burnup MOX)
Figure 7-17 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6 (Low burnup MOX)
Figure 7-18 CTF with IFRAP=0 vs. FRAAPTRAN Fuel Temperature Comparisons for Rod 7 (High burnup MOX)
Figure 7-19 CTF with IFRAP=1 vs. FRAAPTRAN Fuel Temperature Comparisons for Rod 7 (High burnup MOX)
Figures 7-20 and 7-21 show the temperature comparisons for Rod 10, which is a low burnup UO$_2$ fuel rod. Figure 7-20 shows the comparisons for CTF with the IFRAP=0 option. It is seen from the gap conductance plot that in the middle part of the fuel rod FRAPTRAN has a higher gap conductance than CTF since FRAPTRAN gap conductance model takes into account the thermal expansion of fuel pellet. It is seen from the fuel temperature comparisons between CTF and FRAPTRAN that CTF has higher temperature predictions than FRAPTRAN in the middle section of the fuel rod. This higher prediction is due to the fact that CTF has lower gap conductance than FRAPTRAN. Since Rod 10 is a low burnup rod where the burnup level is 0.15 GWD/MTU, the impact of the difference in fuel thermal conductivity models on temperature predictions is low, because MATPRO-11 and the Modified/NFI model predict the same fuel thermal conductivities at low burnups.

Figure 7-21 shows the Rod 10 temperature predictions by CTF with the IFRAP=1 option. When Figure 7-20 and 7-21 is compared, it is seen that fuel centerline temperatures in the middle section is improved.

Figures 7-22 and 7-23 show the temperature comparisons for Rod 11, which is a high burnup UO$_2$ fuel rod. Figure 7-22 shows the comparisons for CTF with the IFRAP=0 option. It is seen from the gap conductance plot that in the middle part of the fuel rod both codes use the same gap conductance. In Figure 7-22, a significant difference between CTF and FRAPTRAN fuel temperature predictions are observed. The differences seen in FRAPTRAN and CTF temperature predictions are due to the difference in the fuel thermal conductivity model of the two codes. CTF with the IFRAP=0 option uses the MATPRO-11 model, whereas FRAPTRAN uses the Modified NFI fuel thermal conductivity model for UO$_2$ fuel. It is seen from fuel temperature prediction comparisons that CTF always underpredicts the fuel centerline and fuel average temperatures when using the IFRAP=0 option. The fuel surface temperature predictions of the two codes are exactly the same since both use the same gap conductance values in the middle section of the rod, where the power is the highest. It is demonstrated that the difference in the gap conductance values in the upper and lower part of the fuel rod, where the power is lowest, do not play a
significant role in the surface temperature predictions. Figure 7-23 shows fuel temperature predictions by CTF using the IFRAP=1 option, which uses the Modified NFI model for UO₂ rods. It is seen from Figure 7-23 that using the IFRAP=1 option in CTF clearly improves the predictions and agrees quite well with the FRAPTRAN predictions.

Figure 7-24 shows the comparisons of the fuel average and the fuel centerline temperature predictions of FRAPTRAN and both CTF options, IFRAP=0 and IFRAP=1, for all rod types. The plots on the top give the predictions of CTF with the IFRAP=0 option and the plots down give the predictions of CTF with the IFRAP=1 option. The deviations in the fuel temperature predictions are seen clearly from Figure 7-24 such that CTF with IFRAP=0 always predicts lower fuel temperatures since the MATPRO-11 model in CTF/IFRAP=0 does not take into account the burnup degradation of fuel conductivity and the MOX fuel properties, which results in a higher fuel thermal conductivity and lower temperature predictions. This effect is not significant for low burnup UO₂ fuel rod though since CTF/IFRAP=0 predicts close results to FRAPTRAN for low burnup UO₂ fuel rod. CTF with the IFRAP=1 option predictions in Figure 7-24 proves the improvement in temperature predictions as results are closer to FRAPTRAN predictions.

Figure 7-25 shows the radial power profiles and Figure 7-26 shows the axial power profile used for all rods types both in FRAPTRAN and CTF calculations. The radial and the axial power profiles embedded into CTF base decks are coming from the FRAPTRAN output files. FRAPTRAN radial and axial power profiles are input to the code and coming from the FRAPCON restart files.
**Figure 7-20** CTF with IFRAP= 0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10 (Low burnup UO₂)
Figure 7-21 CTF with IFRAP=1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10 (Low burnup UO$_2$)
Figure 7-22 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11 (High burnup UO₂)
Figure 7-23 CTF with IFRAP=1 vs. FRAFTRAN Fuel Temperature Comparisons for Rod 11 (High burnup UO$_2$)
Figure 7-24 CTF vs. FRAPTRAN Fuel Temperature Comparisons for All Rods
Figure 7-25 CTF vs. FRAPTRAN RPD for All Rods
7.2.2.2 Steady State Fuel Temperature Comparisons using the Dynamic Gap Conductance in CTF

This section summarizes the fuel temperature predictions by CTF/TORT-TD with IFRAP=0 and IFRAP=1 options when CTF uses the dynamic gap conductance model. This section also compares the fuel temperature predictions from the two models to the CTF/TORT-TD/FRAPTRAN predictions for the configuration shown in Figure 7-13.

The same type of CTF calculations as in section 7.2.2.1 are performed but now using the dynamic gap conductance model to investigate the impact of axially varying gap conductance on the fuel centerline temperatures. Figures 7-27 through Figure 7-34 show the comparisons of the fuel temperature predictions for rod 6, 7, 10 and 11, respectively.

It is seen from the gap conductance plots that there is a difference between CTF and FRAPTRAN calculated gap conductance values. The reason for the observed differences is that CTF does not include burnup dependent fuel rod models such as fuel swelling and densification which will have an impact on the physical gap. In addition to that as burnup changes FRAPTRAN updates the gap gas compositions
whereas CTF does not do it during the calculations. More detailed discussions for the observed differences in gap conductance are provided in the conclusions at the end of this chapter.

When fuel temperature predictions by CTF with the IFRAP=1 option for each rod are compared to the predictions by CTF with the IFRAP=1 option in section 7.2.2.1, where a constant gap conductance is used, it is seen that using the dynamic gap conductance improves the predictions. Although there is not a significant difference between the temperature predictions from the two cases, it is recommended that CTF users should use the dynamic gap conductance model built in CTF.

In summary, CTF/IFRAP=1 results from section 7.2.2.1 and 7.2.2.1 demonstrates that the new burnup dependent fuel rod model implemented in CTF improves the fuel centerline temperature predictions significantly whether the code is using a constant or a dynamic gap conductance model.
Figure 7-27 CTF with IFRAP= 0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6
Figure 7-28 CTF with IFRAP= 1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 6
Figure 7-29 CTF with IFRAP=0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 7
Figure 7-30 CTF with IFRAP= 1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 7
Figure 7-31 CTF with IFRAP= 0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10
Figure 7-32 CTF with IFRAP= 1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 10
Figure 7-33 CTF with IFRAP= 0 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11
Figure 7-34 CTF with IFRAP= 1 vs. FRAPTRAN Fuel Temperature Comparisons for Rod 11
Figure 7-35 CTF vs. FRAPTRAN Fuel Temperature Comparisons for All Rods
Table 7-20 shows the comparisons of neutron multiplication factors $k_{\text{eff}}$ as predicted by the CTF/TORT-TD with the IFRAP=0 option in CTF, the CTF/TORT-TD with the IFRAP=1 option in CTF, and the CTF/TORT-TD/FRAPTRAN coupled systems. It is seen from these results that neutron multiplication factor predicted by TORT-TD when using CTF/IFRAP=1 for fuel temperature feedback gives closer results to the predictions by TORT-TD with feedback from FRAPTRAN. CTF with the IFRAP=0 option underpredicts the fuel temperature, which leads to an overprediction in $k_{\text{eff}}$. The multiplication factor predicted with CTF/IFRAP=1 gives very close result to FRAPTRAN since the fuel temperature predictions with the IFRAP=1 option is improved and very close to the FRAPTRAN predictions.

Table 7-21 and Table 7-22 summarize the statistics for the two CTF options. When the two statistical results are compared it is seen that CTF with the IFRAP=1 option gives better statistical results with a low standard deviation and a higher mean close to 1.00.

Conclusions from Section 7.2 multi-channel steady state cases are as follows:

1) CTF/TORT-TD with IFRAP=1 option gives consistent results with CTF/TORT-TD/FRAPTRAN code for steady state multi-channel configuration demonstrating that CTF with the new fuel thermal conductivity model can model the fuel rod as well as FRAPTRAN; therefore, CTF/TORT-TD with IFRAP=1 calculations can be carried out instead of CTF/TORT-TD/FRAPTRAN calculation to save computational time and simplify the process.

2) CTF/TORT-TD with IFRAP=0 option underpredicts fuel centerline temperature relative to CTF with IFRAP=1 and FRAPTRAN predictions as expected since MATPRO-11 fuel thermal conductivity model does not take into account burnup degradation effects.

3) CTF dynamic gap conductance model gives closer results to FRAPTRAN fuel centerline predictions. For this reason, it is recommended that CTF users use dynamic gap conductance model instead of constant gap conductance model.
4) It is seen from the gap conductance plots in Figure 7-16 through 7-21 that CTF calculated gap conductance values for low burnup fuel rods, Rod 6 (Figure 7-27 and Figure 7-28) and Rod 10 (Figure 7-31 and Figure 7-32) are higher than FRAPTRAN calculated gap conductance values. The reason for this higher prediction is that CTF does not have the densification model, which occurs during low burnup so the physical gap between the two codes is not the same. FRAPTRAN has a higher physical gap due to densification resulting in lower gap conductance. In contrast to Rod 6 and Rod 10, CTF has a lower prediction on gap conductance for high burnup fuel rods Rod 7 (Figure 7-29 and Figure 7-30) and Rod 11 (Figure 7-33 and Figure 7-34). The reason for this low prediction is that CTF does not have fuel swelling model which will have an effect on the physical gap. FRAPTRAN has the swelling model which will decrease physical gap and increase gap conductance for high burnup fuel rods.

5) For low burnup fuel rods CTF predicts $10^4$ W/m²·K higher than FRAPTRAN and for high burnup rods FRAPTRAN predicts $6.10^4$ W/m²·K than CTF. Although gap conductance values show differences between CTF and FRAPTRAN, delta temperature across the gap between the two codes do not show a significant difference and around ~20ºK.

6) Gap conductance plot for fresh fuels in Figure 7-27, 7-28 and 7-31, 7-32 show that in the middle part of the rod where the power is highest, a peak in the gap conductance is observed. This is due to the expansion of the fuel pellet at high temperatures. High power levels results in higher temperatures resulting in fuel pellet to expand more.

7) Reactivity difference between CTF/TORT-TD with IFRAP=1 model and CTF/TORT-TD/FRAPTRAN at steady state conditions is -4.5 pcm whereas reactivity difference between CTF/TORT-TD with IFRAP=0 model and CTF/TORT-TD/FRAPTRAN is 105.7 pcm demonstrating that CTF/TORT-TD with IFRAP=1 option gives very close reactivity values to CTF/TORT-TD/FRAPTRAN prediction.
8) When Table 7-21 and Table 7-22 statistical results are compared it is seen that CTF with the IFRAP=1 option gives much better statistical results with a lower standard deviation and a higher mean close to 1.00, reducing the uncertainty in the temperature calculations and improve prediction capabilities.

<table>
<thead>
<tr>
<th>Table 7-20 Multiplication factor results</th>
</tr>
</thead>
<tbody>
<tr>
<td>K(_{\text{eff}}) (unrodded) &amp; 1.10661 &amp; 1.10539 &amp; 1.10544</td>
</tr>
<tr>
<td>Difference from FRAPTRAN [pcm] &amp; ((1.10661-1.10544)/1.10661) (\times 10^5) = 105.7 &amp; ((1.10539-1.10544)/1.10539) (\times 10^5) = -4.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 7-21 Statistics for CTF with IFRAP=0 results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rod Number &amp; Type &amp; Burnup &amp; (T_{\text{center}}) Mean &amp; (T_{\text{center}}) STD &amp; (T_{\text{average}}) Mean &amp; (T_{\text{average}}) STD</td>
</tr>
<tr>
<td>6 &amp; MOX &amp; Low &amp; 0.9299 &amp; 0.0261 &amp; 0.9504 &amp; 0.0189</td>
</tr>
<tr>
<td>7 &amp; MOX &amp; High &amp; 0.8542 &amp; 0.0469 &amp; 0.9494 &amp; 0.0225</td>
</tr>
<tr>
<td>10 &amp; UO(_2) &amp; Low &amp; 0.9982 &amp; 0.0098 &amp; 0.9850 &amp; 0.0081</td>
</tr>
<tr>
<td>11 &amp; UO(_2) &amp; High &amp; 0.8907 &amp; 0.0363 &amp; 0.9664 &amp; 0.0146</td>
</tr>
<tr>
<td>All rods &amp; &amp; &amp; 0.9182 &amp; 0.0626 &amp; 0.9628 &amp; 0.0223</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 7-22 Statistics for CTF with IFRAP=1 results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rod Number &amp; Type &amp; Burnup &amp; (T_{\text{center}}) Mean &amp; (T_{\text{center}}) STD &amp; (T_{\text{average}}) Mean &amp; (T_{\text{average}}) STD</td>
</tr>
<tr>
<td>6 &amp; MOX &amp; Low &amp; 0.9726 &amp; 0.0254 &amp; 0.9685 &amp; 0.0183</td>
</tr>
<tr>
<td>7 &amp; MOX &amp; High &amp; 1.0171 &amp; 0.0129 &amp; 1.0193 &amp; 0.0075</td>
</tr>
<tr>
<td>10 &amp; UO(_2) &amp; Low &amp; 0.9839 &amp; 0.0157 &amp; 0.9805 &amp; 0.0116</td>
</tr>
<tr>
<td>11 &amp; UO(_2) &amp; High &amp; 1.0093 &amp; 0.0086 &amp; 1.0142 &amp; 0.0053</td>
</tr>
<tr>
<td>All rods &amp; &amp; &amp; 0.9957 &amp; 0.0247 &amp; 0.9956 &amp; 0.0246</td>
</tr>
</tbody>
</table>
7.3 References


CHAPTER 8  

ROD EJECTION ACCIDENT TRANSIENT RESULTS  

Chapter 8 summarizes the rod ejection accident (REA) transient results performed by using the 4x4 PWR array configuration used in Chapter 7. REA transient is simulated by starting at Hot-Zero-Power (HZP) and also at Hot-Full-Power (HFP) conditions with control rod in a half inserted position. Both scenarios are analyzed by CTF/TORT-TD with IFRAP=0 and IFRAP=1 options and results are compared against CTF/TORT-TD/FRAPTRAN predictions. Power pulse and fuel average temperature increase during the transient is investigated to see the impact of thermal conductivity degradation (TCD) on the Doppler feedback effect.

Section 8.1 gives background information on rod ejection accident transients before results are analyzed.

Section 8.2 demonstrates the HZP REA results generated by CTF/TORT-TD with IFRAP=1 and IFRAP=0 options. Results are compared against the same cases run on CTF/TORT-TD/FRAPTRAN coupled code. Sensitivity studies are performed with CTF/TORT-TD to see the impact of radial power distribution and gap conductance on the power pulse and fuel temperature plots.

Section 8.3 demonstrates the HFP REA results generated by CTF/TORT-TD with IFRAP=1 and IFRAP=0 options. Power pulse, fuel average temperature increase and enthalpy rise plots are generated by CTF with IFRAP=0 and IFRAP=1 option using dynamic gap conductance and FRAPTRAN-based radial power distributions (RPD). IFRAP=1 and IFRAP=0 results are compared against each other to see the impact of TCD model on the Doppler feedback effect and power spike.

Section 8.4 summarizes the observations and conclusions from section 8.2 and 8.3.

8.1 Background

The Rod Ejection Accident (REA) is accepted as a design basis Reactivity Initiated Accident (RIA) for PWRs [1,2,3,4]. It might occur due to mechanical failure of control rod drive mechanism or
pressure housing unit. The control rod and drive tube might be ejected due to pressure difference between the reactor coolant system and containment. As a result of this, a rapid positive reactivity insertion is introduced into the reactor, which results in a core power spike in milliseconds that might lead to fuel rod damage by fuel pellet overheating and thermal expansion. The reactor exceeds prompt criticality threshold and reaches in super prompt critical state, all the fuel rods experience heat-up due to rapid core power increase and fuel pellets might come into contact with the cladding inner wall and also increase local stress and strain, as a result, cladding might fail due to excessive pellet-cladding mechanical interaction (PCMI).

During this transient, the fuel negative temperature coefficient of reactivity or the fuel Doppler reactivity coefficient (DRC) can turn the reactor core power increase downward. In a typical light water moderated reactor, this coefficient is negative and is the result of the Doppler Effect, which is also called Doppler broadening. Increasing fuel temperature makes the nuclei vibrate more rapidly within their lattice structure that effectively broadens the energy range of neutrons that might be absorbed in the fuel resonances. This broadening will increase the total number of neutrons absorbed by the large resonances of fuel heavy uranium material such as U-238 while also reducing the resonance escape probability. This will reduce the multiplication factor or eigenvalue of the system based on 6-factor formula calculation [5]. This mechanism introduces more negative reactivity into the reactor at higher temperatures that will eventually compensate the initial positive reactivity insertion in REA accident. This behavior is much more important than a negative moderator temperature coefficient due to the fact that fuel temperature quickly increases following a reactor power increase. In the event of a large positive reactivity insertion such as REA accident, moderator temperature coefficient becomes a secondary important factor and cannot contribute to overcome the power increase for several seconds, however, fuel temperature coefficient injects negative reactivity into system immediately. In other terms, generated energy by the power rise is stored quickly in the fuel and then released to the rest of the system.
8.2 HZP REA Results

Sensitivity studies are performed by using uniform and FRAPTRAN-based RPDs with constant and dynamic gap conductance options to investigate which combination of the models would give closer results to FRAPTRAN predictions. HZP REA is simulated by CTF/TORT-TD with IFRAP=0 and IFRAP=1 option and results are compared against the same case run on CTF/TORT-TD/FRAPTRAN coupled code.

Table 8-1 summarizes HZP REA output parameters for the three fuel rod models based on steady state calculations. The calculated total half-rod reactivity worth is 835 pcm with a total $1.156 positive reactivity insertion during the transient for all the models.

<table>
<thead>
<tr>
<th>HZP Parameter</th>
<th>CTF/TORT-TD IFRAP=0</th>
<th>CTF/TORT-TD IFRAP=1</th>
<th>CTF/TORT-TD FRAPTRAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{eff}$ (unrodded)</td>
<td>1.12059</td>
<td>1.12059</td>
<td>1.12059</td>
</tr>
<tr>
<td>$k_{eff}$ (half-rodded)</td>
<td>1.11123</td>
<td>1.11123</td>
<td>1.11123</td>
</tr>
<tr>
<td>Half-rod reactivity worth (pcm)</td>
<td>$(1.12059- 1.1123)/1.12059 *10^{-5}= 835.3$</td>
<td>$(1.12059- 1.1123)/1.12059 *10^{-5}= 835.3$</td>
<td>$(1.12059- 1.1123)/1.12059 *10^{-5}= 835.3$</td>
</tr>
<tr>
<td>Reactivity (unrodded)</td>
<td>0.1076129</td>
<td>0.1076129</td>
<td>0.1076129</td>
</tr>
<tr>
<td>Reactivity (half-rodded)</td>
<td>0.1000963</td>
<td>0.1000963</td>
<td>0.1000963</td>
</tr>
<tr>
<td>Total positive reactivity insertion</td>
<td>$7.5166*10^{-3}$</td>
<td>$7.5166*10^{-3}$</td>
<td>$7.5166*10^{-3}$</td>
</tr>
<tr>
<td>Total positive reactivity insertion ($$$)</td>
<td>1.156</td>
<td>1.156</td>
<td>1.156</td>
</tr>
</tbody>
</table>

Figure 8-1 shows the power spike, fuel average temperature and fuel maximum temperature during the REA transient when uniform RPD and constant gap conductance is used. The constant gap conductance values and the fuel configuration used in these calculations are the same with Section 7.2.2.1. Figure 8-1 shows that power spike and temperature predictions from CTF with IFRAP=0 and IFRAP=1 options are very close to FRAPTRAN predictions. Since uniform RPD is used, CTF prediction at the spike is slightly higher (~4 MW more) than FRAPTRAN prediction which is 66 MW.
It is noticed that there is no difference between CTF with IFRAP=0 and IFRAP=1 predictions. No impact of TCD is observed at HZP REA power spike and fuel temperature results. The reason for this behavior is that the transient starts from a HZP condition where there is negligible power in the system. Moderator and fuel temperatures are close to each other around 560ºK, transient is fast (60 milliseconds) and there is not enough time for heat removal from the system to be able to see the impact of TCD.

Figure 8-1 fuel average temperature vs. time plot shows that CTF and FRAPTRAN almost predict the same fuel average temperature. When fuel maximum temperatures are compared it is seen that CTF predicts higher temperatures than FRAPTRAN since CTF/TORT-TD predicts total bundle power higher than CTF/TORT-TD/FRAPTRAN. Temperature predictions shown in Figure 8-1 are obtained from the TORT-TD output file, where TORT-TD does volume weighted averaging on the fuel.

Figure 8-2 shows the transient results when CTF uses uniform RPD and dynamic gap conductance model. It is seen from the power evolution plot in Figure 8-2 that when dynamic gap conductance model is used, power spike drops from 70 MW to 64 MW compared to Figure 8-1 and gets slightly lower than FRAPTRAN power spike which is 66 MW.

Figure 8-3 shows the transient results when CTF uses FRAPTRAN-based RPD and constant gap conductance. It is noticed from Figure 8-3 that when FRAPTRAN-based RPD is used in CTF calculations, power peak drops to 60 MW. The use of FRAPTRAN-based RPD has an additional impact of 4 MW drop in the power spike.

Figure 8-4 shows the transient results when CTF uses FRAPTRAN-based RPD and dynamic gap conductance. It is noticed from Figure 8-4 that power peak drops to 50 MW, which is 10 MW lower than CTF predictions in Figure 8-3. This is the lowest of peak in all of the four scenarios.

Although in steady state calculations which started from HFP state in Section 7.2.2.2, using a FRAPTRAN-based RPD and a dynamic gap conductance predicted the best estimate temperature predictions, the same behavior is not observed in HZP REA. This is due to the fact that transient starts at
HZP conditions and it is difficult to simulate the impact of TCD in 60 milliseconds transient at zero power. Therefore, a HFP transient is needed to perform to demonstrate the impact of TCD on the transient results, which will be discussed in the next section.
Figure 8-1 REA Transient Results at HZP condition, CTF uses uniform RPD and constant hgap
Figure 8-2 REA Transient Results at HZP condition, CTF uses uniform RPD and dynamic hgap
Figure 8-3 REA Transient Results at HZP condition, CTF uses FRAPTRAN RPD and constant hgap
Figure 8-4 REA Transient Results at HZP condition, CTF uses FRAPTRAN RPD and dynamic hgap
8.3 HFP REA Results

Section 8.3 discusses HFP REA results. The same fuel configuration in section 8.2 is used and the same transient is simulated by CTF/TORT-TD with IFRAP=0 and IFRAP=1 option at HFP conditions. Transient is started from HFP conditions where fuel and moderator temperatures are at nominal operating conditions and initial 4x4 pin-array power is 1.04952 MW. FRAPTRAN-based RPD and dynamic gap conductance model is used in CTF/TORT-TD simulations.

It is demonstrated in the previous chapters that CTF with TCD model (IFRAP=1) predicts higher temperatures compared to CTF without TCD model (IFRAP=0). HFP REA transient starting temperatures will be different between IFRAP=0 and IFRAP=1 option. Before analyzing the results, an alternate calculation is performed to demonstrate the impact of different starting fuel temperatures on the prompt Doppler coefficient based on the Equation 8-1 [5].

\[
\alpha_{\text{prompt}} = \frac{\beta_1}{2\sqrt{T}} \ln \left[ \frac{1}{p(300 \text{ K})} \right] \quad \text{(Equation 8-1)}
\]

Where \(\beta_1\) is a fuel dependent constant and \(p\) is the resonance escape probability at 300ºK and constant for different temperatures. They are same for the same fuel type and \(\alpha_{\text{prompt}}\) becomes inversely proportional with the square root of the temperature. One can calculate the prompt temperature coefficient change for different temperatures. Table 8-2 summarizes the sensitivity study results to better understand the impact of two different starting temperatures on the Doppler reactivity coefficient. For example, when the fuel temperature is higher as it is in the case with CTF IFRAP=1 option, \(\alpha_{\text{prompt}}\) gets less negative. Inversely, when fuel temperature is lower as it is in the case with CTF IFRAP=0 option, \(\alpha_{\text{prompt}}\) gets more negative.
### Table 8-2 Alternate Calculation Summary for Doppler Reactivity Coefficient

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Fuel temperature (ºK)</th>
<th>Delta temperature increase (ºK)</th>
<th>$\alpha_{\text{prompt}}$ (1/ºC or ºK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Reference</td>
<td>623</td>
<td>0</td>
<td>$-1.390 \times 10^{-5}$</td>
</tr>
<tr>
<td>Case 1</td>
<td>723</td>
<td>100</td>
<td>$-1.282 \times 10^{-5}$</td>
</tr>
<tr>
<td>Case 2</td>
<td>1123</td>
<td>500</td>
<td>$-1.028 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Figure 8-5 shows total power spike during REA HFP transient. It is seen from Figure 8-5 that CTF/IFRAP=1 has a power spike around 35 MW which is higher than CTF/IFRAP=0. The higher spike observed in CTF/IFRAP=1 option is due to the fact that the prompt temperature coefficient is less negative at elevated temperatures. Since IFRAP=1 is going to predict higher fuel temperatures than IFRAP=0 option, the resulting Doppler coefficient will be less negative, resulting in a higher power pulse.

Figure 8-6 shows weighted fuel average temperature profile during the transient. It is seen from Figure 8-6 that CTF/IFRAP=1 has higher temperatures since it has higher total power compared to CTF/IFRAP=0.

Figure 8-7 demonstrates peak nodal fuel enthalpy deposition during the transient for CTF IFRAP=0 and IFRAP=1 option. It is seen from Figure 8-7 that the initial enthalpy is around 40 cal/gr and it goes up to 60 cal/gr at the end of the transient. It is noticed that IFRAP=1 has a higher energy deposition than IFRAP=0 but the difference between the two curves is not significant because the delta temperature increase during the transient between the two models are almost the same as demonstrated in Figure 8-13 and 8-14. Also, both values are well below the limit of ~100 cal/gr for fuel failure in high burnup [6].

To investigate the difference in the starting fuel temperatures between the two models, one high burnup UO₂ (rod 7) and one high burnup MOX fuel rod (rod 11) are selected from the PWR 4x4 fuel array shown previously in Figure 7-13.
Figures 8-8 to 8-11 demonstrate the fuel centerline temperature profiles during the transient for Rod 7 and Rod 11. For the high burnup MOX fuel rod (Rod 7), maximum fuel centerline temperature is around 2000ºK with IFRAP=0 model whereas it goes up to around 2500ºK with the IFRAP=1 model (experiencing a 500ºK temperature difference). The similar behavior is observed for the high burnup UO₂ fuel rod (Rod 11). The maximum fuel centerline temperature is around 1700ºK with IFRAP=0 model and 2000ºK with the IFRAP=1 model during the transient (experiencing 300ºK temperature differences). Figures 8-8 through 8-11 confirm that REA HFP transient starts at two different temperatures between the two CTF models.

Figures 8-12 shows the difference in the fuel centerline temperature predictions for Rod 7 between CTF IFRAP=0 and IFRAP=1 models. Almost 500ºK fuel centerline temperature difference is observed during the transient at the peak node.

Figure 8-13 demonstrates the temperature increase during the transient for high burnup MOX rod when CTF with IFRAP=0 option is used. Figure 8-14 demonstrates the temperature increase during the transient for high burnup MOX rod when CTF with IFRAP=1 option is used. When the delta temperature increase at the peak node (which is between 0.5m to 1.0 m axial position) is compared between the two models, it is seen that the delta temperature increase at the peak node during the transient is around 80ºK in both of the models.

Table 8-3 summarizes HFP parameters such as multiplication factor, control rod worth and reactivity inserted into the system. It is shown that the total reactivity insertion to the system in both of the CTF models is the same and $1.66.

It is concluded from HFP REA transient analysis that when the same amount of positive reactivity insertion is applied to the two systems with two different temperatures, the system with higher temperatures will experience a less negative reactivity feedback and end up with a higher
power spike. As temperature increases during the transient due to the Doppler feedback effect the power spike is eventually going to go down.

**Table 8-3** HFP output parameters for the two CTF models

<table>
<thead>
<tr>
<th>HFP Parameter</th>
<th>CTF/TORT-TD IFRAP=0</th>
<th>CTF/TORT-TD IFRAP=1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{eff}$ (unrodded)</td>
<td>1.10661</td>
<td>1.10539</td>
</tr>
<tr>
<td>$k_{eff}$ (half-rodded)</td>
<td>1.09355</td>
<td>1.09239</td>
</tr>
<tr>
<td>Half-rod reactivity worth (pcm)</td>
<td>((1.10661- 1.09355)/1.10661) *10^{-5}= 1180</td>
<td>((1.10539-1.09239)/1.10539) *10^{-5}= 1176</td>
</tr>
<tr>
<td>Reactivity (unrodded)</td>
<td>0.096339</td>
<td>0.0953419</td>
</tr>
<tr>
<td>Reactivity (half-rodded)</td>
<td>0.08554</td>
<td>0.08457</td>
</tr>
<tr>
<td>Total positive reactivity insertion</td>
<td>0.010799</td>
<td>0.0107719</td>
</tr>
<tr>
<td>Total positive reactivity insertion ($)</td>
<td>1.662</td>
<td>1.657</td>
</tr>
</tbody>
</table>

![Figure 8-5](image-url) **Figure 8-5** REA Transient Total Power Results at HFP condition
Figure 8-6 REA Transient Fuel Average Temperature Results at HFP condition

Figure 8-7 REA Peak Fuel Enthalpy
Figure 8-8 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 7 (IFRAP=0)

Figure 8-9 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 7 (IFRAP=1)
Figure 8-10 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 11 (IFRAP=0)

Figure 8-11 REA Transient Fuel Centerline Temperature Results at HFP condition for Rod 11 (IFRAP=1)
**Figure 8-12** REA Transient Fuel Centerline Temperature Differences at HFP condition for Rod 7

**Figure 8-13** Delta ta Fuel Centerline Temperature for Rod 7 during HFP REA using CTF with IFRAP=0
Figure 8-14 Delta ta Fuel Centerline Temperature for Rod 7 during HFP REA using CTF with IFRAP=1

8.4 Conclusions

1. At HZP steady state condition, CTF predicted power spike and temperature values are very close to FRAPTRAN predictions when CTF uses constant gap conductance and uniform RPD. Using dynamic gap conductance model in CTF leads to an under prediction in the power spike. CTF with IFRAP=0 and IFRAP=1 options give the same power spike and temperature values confirming that there is no impact of TCD at HZP conditions.

2. HFP REA transient analysis shows that CTF with IFRAP=1 option predicts a higher power spike and thus a higher fuel temperature compared to CTF with IFRAP=0 option. The reason for this behavior is that prompt temperature coefficient is less negative at
elevated temperature as it is the case in CTF with IFRAP=1 option. Less negative Doppler coefficient results in a higher power spike.

3. Peak fuel enthalpy plot shows that enthalpy increase during the HFP transient is 60 cal/gr. CTF with IFRAP=1 option has a higher enthalpy deposition than IFRAP=0 option since IFRAP=1 option has higher temperature predictions.

4. CTF with the TCD model (IFRAP=1) predicts lower thermal conductivity for high burnup fuels that causes higher fuel centerline temperature predictions when compared to CTF with IFRAP=0 option. It is observed that REA starts at almost 500ºK higher temperature at the peak node with IFRAP=1 option.

5. At HFP REA transient analysis, CTF/IFRAP=1 has a power spike around 35 MW which is 13 MW higher than CTF/IFRAP=0. The higher spike observed in CTF/IFRAP=1 option is due to the fact that the prompt temperature coefficient is less negative at elevated temperatures. Since IFRAP=1 is going to predict higher fuel temperatures than IFRAP=0 option, the resulting Doppler coefficient will be less negative resulting in a higher power pulse. The impact of fuel conductivity degradation is more visible at HFP transient calculations. CTF without the TCD model (IFRAP=0), not only predicts lower and incorrect power spike but also it predicts the power spike in a non-conservative direction. On the other hand, the fuel thermal conductivity degradation model (IFRAP=1) improves the prediction capabilities of CTF in a conservative direction during the transient.
8.4 References


CHAPTER 9

CONCLUSIONS AND FUTURE WORK

9.1 Conclusions

The main outcome from this PhD dissertation is the development and implementation of a fuel thermal conductivity degradation (TCD) model in the CTF/TORT-TD coupled code system as a new option. An input called IFRAP was created to invoke the new fuel thermal conductivity model in CTF. IFRAP=0 uses the traditional MATPRO-11 fuel properties model and IFRAP=1 uses the new thermal conductivity degradation model in CTF.

A new improved high fidelity tool CTF/TORT-TD with IFRAP=1 option was developed for practical safety analysis and faster steady-state and transient calculations. CTF/TORT-TD with IFRAP=1 option not only provides more efficient calculations when compared to CTF/TORT-TD/FRAPTRAN, but it also gives better prediction capability of fuel centerline temperatures as compared to experimental data. In other words, it combines accuracy with efficiency.

Fuel centerline temperature is a licensing criterion in nuclear reactors and it is very important to predict the fuel centerline temperature (TCL) accurately since it is going to affect results of several safety analyses. In October 2009, the Nuclear Regulatory Commission (NRC) issued an information notice (IN 2009-23) to all fuel vendors [1]. IN 2009-23 was issued to notify the holders of operating licenses about the impact of nuclear fuel thermal conductivity degradation. NRC expected all the recipients of the IN 2009-23 to review the information and consider actions for their facility. It is indicated in IN 2009-23 that licensees use a series of computer codes to analyze plant behavior in safety analysis to demonstrate that they meet the applicable regulatory criteria. Within the scope of reload licensing evaluations, licensees use these computer codes to establish cycle operating limits to ensure that all applicable requirements
(e.g., fuel thermal-mechanical limits, core thermal-hydraulic limits, emergency core cooling system limits, and nuclear design limits) are met. If fuel thermal conductivity is not calculated correctly then the calculated margins or other limits may be less conservative than previously understood. With the development of CTF/TORT-TD with IFRAP=1 option, thermal conductivity will be calculated correctly and safety analysis performed using this tool will give best-estimate results, which can be used to establish margins and/or limits.

Different steps were taken within the course of this work. First, a sensitivity study was performed to investigate the radial fuel rod thermal behavior. 1D heat conduction equation was solved analytically and four fuel parameters: fuel pellet conductivity, gap conductance, fuel pellet radius, and clad inside radius were changed and effect of each parameter on the fuel radial temperature profile was investigated. It was demonstrated that the fuel thermal conductivity and the gap conductance are the two major parameters changing the fuel radial temperature profile.

Second, sensitivity analyses were performed on the modified NFI model by changing the exposure and the gadolinium concentrations to create a thermal conductivity database and it was compared to the current MATPRO-11 model in CTF. Thermal conductivity versus fuel centerline temperatures were plotted to demonstrate the fuel thermal conductivity degradation with exposure and Gd increment and results were compared to MATPRO-11 model predictions. It was demonstrated that both models predict very close conductivity values at 0 GWd/MTU and 0 Gadolina w/o concentration.

Third, the modified NFI fuel thermal conductivity model was integrated into CTF with a new option called IFRAP=1 and predicted fuel thermal conductivities were benchmarked against FRAPCON-3.4 predictions. It was demonstrated that the new TCD model in CTF predicts the same thermal conductivities as FRAPCON-3.4.
Forth, the fuel centerline temperatures predicted by CTF with the new TCD model (IFRAP=1) were validated against the Halden experimental test data and FRAPCON-3.4 predictions. Experimental test cases from Halden reactor for UO₂ fuel rods at Beginning of Life (BOL), through lifetime without Gd₂O₃, and a MOX fuel rod were simulated with CTF. It was demonstrated that CTF with the new TCD model (IFRAP=1) predicts fuel centerline temperature within 10% uncertainty band as compared to experimental data.

After implementing the new thermal conductivity model in CTF and validating the model with experimental data, CTF with IFRAP=1 model was applied to steady state and transient calculations by using 4x4 PWR fuel bundle configuration from Purdue MOX benchmark. First, one of each high burnup UO₂ and MOX fuel rods from 4x4 matrix was selected to carry out single fuel rod calculation. Fuel centerline temperatures predicted by CTF/TORT-TD were compared against CTF/TORT-TD/FRAPTRAN predictions. After confirming that the new TCD model in CTF works properly and gives consistent results with FRAPTRAN predictions for a single fuel rod configuration, the same type of analysis was carried out for a bigger system which is a 4x4 PWR pin-array consisting of 15 fuel pins and one control guide tube.

Steady state calculations at Hot Full Power (HFP) conditions were performed using the 4x4 PWR pin-array with CTF/TORT-TD coupled code system. Fuel centerline, surface and average temperatures predicted by CTF/TORT-TD with and without TCD model were compared against CTF/TORT-TD/FRAPTRAN predictions. It was demonstrated that CTF/TORT-TD with IFRAP=1 can be carried out instead of CTF/TORT-TD/FRAPTRAN. Statistical analyses were performed on CTF fuel centerline predictions with and without the TCD model. It was demonstrated that statistics for the fuel centerline temperature predictions were improved with CTF IFRAP=1 option which has 0.9957 mean and 0.0247 standard deviation whereas CTF with IFRAP=0 option has 0.9182 mean and 0.0626 standard deviation.
Moreover, the constant and the dynamic gap conductance models in CTF were used with the TCD model. It was shown that the CTF dynamic gap conductance model, which uses cold gap width and mole fraction of the gas compositions in the gap as an input, had a higher prediction capability on fuel centerline and surface temperatures when compared to constant gap conductance model. It was demonstrated that the CTF dynamic gap conductance model performs as well as the FRAPTRAN gap conductance model. In high burnup rods, since gap conductance (h_{gap}) is so high (10^5 \text{ W/m}^2\text{-ºK}), the effect of h_{gap} decreases and therefore a constant h_{gap} can be used in calculations. The effect of h_{gap} decreases at high burnup whereas the effect of thermal conductivity degradation increases. At low burnup, using TCD model becomes less important but the effect of using dynamic h_{gap} increases.

The impact of CTF TCD model on the core reactivity calculations was demonstrated. Reactivity difference between CTF/TORT-TD with IFRAP=1 model and CTF/TORT/FRAPTRAN at steady state conditions is -4.5 pcm whereas reactivity difference between CTF/TORT-TD with IFRAP=0 model and CTF/TORT/FRAPTRAN is 105.7 pcm, which demonstrates that CTF/TORT-TD with IFRAP=1 option gives closer reactivity predictions to CTF/TORT/FRAPTRAN.

Finally, a Rod Ejection Accident (REA) scenario using the same 4x4 PWR pin-array was simulated both at Hot Zero Power (HZP) and HFP conditions, starting from half of the control rod inserted position. The two scenarios were run using CTF/TORT-TD coupled code system with and without the TCD model. The purpose of this transient analysis was to show the impact of TCD on feedback effects, specifically Doppler Reactivity Coefficient (DRC) and eventually on total core reactivity during the transient.

For HZP REA transient analysis, power spike and temperature predictions from CTF were very close to FRAPTRAN predictions when uniform RPD and constant gap conductance
models were used. Since uniform RPD was used, CTF predictions at the spike were slightly higher (~4 MW more) than FRAPTRAN prediction which was 66 MW. It was noticed that there was no difference between CTF with IFRAP=0 and IFRAP=1 predictions. No impact of TCD was observed at HZP REA power spike and fuel temperature results. The reason for this behavior was that the transient started from a HZP condition where there was negligible power in the system. Moderator and fuel temperatures were close to each other around 560ºK, transient was fast (60 milliseconds) and there was not enough time for heat removal from the system to be able to see the impact of TCD. In addition to that, the initial starting temperatures between the two CTF models were different when transient started. CTF with IFRAP=1 option started with almost 500ºK higher at the peak node when compared to CTF with IFRAP=0. Temperature increase at the peak node during the transient was around 80ºK in both of the CTF models.

For HFP REA transient analysis, CTF/IFRAP=1 had a power spike around 35 MW which was 13 MW higher than CTF/IFRAP=0. The higher spike observed in CTF/IFRAP=1 option was due to the fact that the prompt temperature coefficient was less negative at elevated temperatures. Since IFRAP=1 was going to predict higher fuel temperatures than IFRAP=0 option, the resulting Doppler reactivity coefficient would be less negative resulting in a higher power pulse. The impact of TCD was more visible in HFP transient calculations. CTF without the TCD model (IFRAP=0), not only predicted lower and incorrect power spike but also in a non-conservative direction. On the other hand, the fuel thermal conductivity degradation model (IFRAP=1) improved the prediction capabilities of CTF in a conservative direction and also gave more accurate results during the transient.
9.2 Summary of Contributions

The original PhD contribution of this dissertation is the development and validation of TCD model within the subchannel thermal-hydraulics code CTF. The model takes into account first, the degradation of fuel thermal conductivity with high burnup; and second, the fuel thermal conductivity dependence on the Gadolinium and MOX content.

TCD model is implemented and tested in the standalone CTF code and is available to users to perform both steady state and transient analysis. In addition to that the TCD model is integrated into PSU/RDFMG CTF/TORT-TD coupled system code as a new option that can be run in parallel mode. The CTF/TORT-TD can be run for both steady state and transient analysis for safety evaluation calculations. MATPRO-11 model in CTF is kept as an option (IFRAP=0) for backwards compatibility and the new TCD model is available to users as a new option (IFRAP=1).

The new improved high-fidelity tool CTF/TORT-TD with IFRAP=1 developed for practical analysis and faster steady state and transient calculations addresses the effect of burnable poison Gd on fuel temperature distribution, thermal conductivity degradation with high burnup, provides more accurate fuel temperature predictions and improves the computational efficiency as compared to coupled thermal hydraulics/fuel performance codes. The advantage of such coupled system as compared to coupled thermal-hydraulics/neutronics/fuel performance codes is that it has much more computation efficiency, which is of great importance for routine design and safety evaluations performed in industry and regulation.

Moreover, CTF/TORT-TD with IFRAP=1 improves the accuracy of fuel centerline temperature predictions and also improves the feedback modeling during the operational transients and postulated accidents.
The other contribution from this study is that the CTF model can perform TCD calculations on axial nodal basis that provides ability to model axially non-uniform UO₂, UO₂-Gd₂O₃ and MOX fuels whereas fuel performance codes such as FRAPCON/FRAPTRAN only considers axially uniform UO₂, UO₂-Gd₂O₃ and MOX fuels.

Furthermore, CTF also provides thermal conductivity calculation at each axial, radial and azimuthal node (3D representation).

9.3 Suggestions for Future Work

Transient analysis for LOCA and RIA can be simulated to see the impact on TCD on core reactivity. LOCA transient case can be run and its impact on the Peak Clad Temperature (PCT) and fuel centerline (TCL) can be investigated. In addition to that RIA case can be simulated for a BWR rod drop accident and the impact on Doppler reactivity coefficient and fuel moderator coefficient can be investigated.

CTF dynamic gap conductance model can be improved by including the densification and swelling models which will affect the gap width and gap conductivity. Another option is to implement pre-calculated fitting gap conductance tables as function of burnup and power.

Another RIA transient can be run from literature where the peak fuel enthalpy results can be benchmarked.
APPENDIX A

GADOLINIUM OXIDE LATTICE STRUCTURE

Gadolinium oxide (or Gadolina) is also called gadolinium trioxide and can be displayed as gadolinium (III) oxide. It has a molecular formula of Gd₂O₃. It is constituted by the rare earth element of gadolinium and oxygen atoms. Table A-1 summarizes the physical and structural properties of Gadolinium oxide [1]. It has the following crystal structures and lattice types based on operating temperatures: 1) Cubic structure is valid around room temperatures with a body centered lattice type configuration and it is notated by Pearson symbol [2] of cI80, which c and I notations stands for cubic crystal and body centered lattice configuration type, and 80 refers to number of atoms in an equivalent unit cell of gadolinium oxide, 2) Transition and phase change to the monoclinic structure takes place around 1200°C and is observed up to 2100°C (this range is the typical temperatures for nuclear fuel operating conditions). Pearson symbol of gadolinium oxide monoclinic structure is mS30, which m and S notations refers to monoclinic crystal system with side face centered lattice configuration respectively, and 30 refers to number of atoms in an equivalent unit cell of gadolinium oxide. An equivalent unit cell might consist of more than one lattice. The monoclinic crystal lattice system is also described by unequal vector lengths as shown in Figure A-1, 3) Hexagonal phase shifts experienced beyond 2100°C up to melting point of 2420°C. Figure A-1 shows the crystal structures and phase transitions by operating temperatures for gadolinium oxide.

Figure A-2 demonstrates sample cubic lattice configurations [1, 3]. It can be seen in the Figure that the simple cubic lattice configuration system contains one lattice point on each corner of the cube. Each atom is shared equally between eight adjacent cubes, it results with a total of one atom in the unit cell ((1/8)*8=1). The body centered cubic (bcc) configuration holds one lattice point in the center of the unit cell with eight corner points and it has total of 2 lattice points per unit cell ((1/8)*8 + 1=2). Finally,
the face centered cubic (fcc) configuration has lattice points on the faces of the cube contributing one half fraction in addition to corner lattice points, and it has total of 4 lattice points per unit cell ((1/8)*8)=1 from the corners + (1/2)*6=3 from the faces).

### Table A-1 Gadolinium Oxide physical and structural properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar Mass (g/mol)</td>
<td>362.468 g/mole</td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td>7.10 (at room temperature)</td>
</tr>
<tr>
<td>Melting Point (°C)</td>
<td>2420</td>
</tr>
<tr>
<td>Crystal Structure</td>
<td>Cubic (at room temperature)</td>
</tr>
<tr>
<td></td>
<td>Monoclinic (1200 – 2100°C)</td>
</tr>
<tr>
<td></td>
<td>Hexagonal (&gt;2420°C)</td>
</tr>
<tr>
<td>Appearance</td>
<td>White Odorless Powder</td>
</tr>
</tbody>
</table>

![Figure A-1](image1.png)  
**Figure A-1** Demonstration of Gadolinium Oxide Crystal Structures and Phases

![Figure A-2](image2.png)  
**Figure A-2** Sample Demonstration of Cubic Lattice Configurations
A.1 References


APPENDIX B

CTF, FRAPTRAN and TORT-TD THREE CODES COUPLING SYSTEM

CTF, FRAPTRAN and TORT-TD were integrated into a single code by using serial integration techniques with some parallelism for FRAPTRAN calculations in 2013 by Magedanz [1] at Penn State Nuclear Engineering Department. The detailed description of the coupling structure, code interfaces, and information exchanged were given in Magedanz dissertation studies [1]. This study extends to previous work by incorporating the new thermal conductivity model into CTF calculations. Source code modifications occurred within CTF modules have also been incorporated into three code coupling systems mentioned here. The updated version of three code coupling system was recompiled to analyze the impact of the new CTF thermal conductivity model for fully coupled steady state and transient calculations. Therefore, coupling system and information flow between codes is briefly summarized in this section.

The layer abstraction technique was used to separate the main program and each sub codes from each other within object-oriented programming structure [1]. By the help of this method, all the variables within each sub-code were separated and encapsulated from other program access. All communications between the codes occur via “interface” methods. The top level system diagram of the coupling structure is given in Figure B-1. Figure B-1 shows that each interface has a data transfer module sharing its data with the main program and other interfaces.
Figure B-2 shows the data transfer between CTF and FRAPTRAN with TORT-TD feedback. Flow area and wetter perimeter changes due to total heating in the coolant channels which are tightly coupled to fuel rods with changing fuel rod area and perimeter parameter at each time interval. In CTF calculations, the clad temperature is used for determining flow regimes, friction factor and the heat transfer coefficients transferred back to FRAPTRAN calculations. The fuel rods can be modeled in either in CTF or FRAPTRAN and the fuel temperature is extracted from the code that models the fuel rod. TORT-TD power distribution can be transferred to both CTF and FRAPTRAN calculations.
**Figure B-2** Data Transfer between CTF and FRAPTRAN with TORT-TD Feedback

**B.1 References**

APPENDIX C

CTF NUCLEAR FUEL ROD DEFORMATION MODEL

This section summarizes the nuclear fuel rod deformation model available within CTF calculations. In simulating accident conditions in the reactor, the prediction of the fuel centerline temperature becomes very important goal to check it against the fuel material melting point to protect fuel integrity. CTF models UO₂ fuel and Zircaloy cladding with a very thin gap structure between them. Fill gases can be helium, xenon, argon, krypton hydrogen, and nitrogen. Heat conduction takes place in three regions such as 1) Metal cladding with Zircaloy cladding properties used, 2) Thin gap region between the cladding and the fuel pellet with no convection transfer, and 3) Fuel pellet region.

In the gap region, gas conduction and radiation heat transfer between the pellet and cladding inner surfaces are the two dominant heat transfer mechanisms. The fuel pellet temperature profile is calculated by solving the radial heat conduction equation. Fuel pellet dimensions vary due to pellet expansion and contraction during the fuel operation and have impact on gap size and gap heat transfer. In addition, pellet cracking might be observed due to thermal expansion of the fuel. CTF fuel deformation model incorporates these effects into fuel pellet thermal conductivity calculations [1].

C.1 Fuel Pellet Cracking and Sintering Effect on Conductivity

Thermal conductivity of the fuel is reduced by rod fill gas replacing the fuel material in the cracks during the operation caused by fuel expansion and cracking. In CTF [1], thermal conductivity degradation was taken into consideration by incorporating FRACAS-I mechanics model from FRAPCON-2. The model includes a multiplication correction factor, which is a function of the gas conductivity and the cracking volume. CTF theory manual provides detailed information and the correlation for the correction factor and new cracked fuel thermal conductivity. Thermal conductivity degradation effect with cracking disappears near fuel sintering temperature of UO₂ and the multiplication factor is set to 1.0 for the fuel temperatures beyond 4304°F. Figure C-1 shows a sample of cracked uranium oxide fuel.
C.2 Fuel Pellet and Cladding Expansion Effects on Gap Thickness

CTF dynamically considers the thermal expansion of the fuel pellet and thermal and mechanical expansion of the cladding in the calculation of gap thickness. Burnup dependent changes due to swelling and densification are not modeled. Mechanical stress is imposed on the cladding due to differences between fill gas and system pressures for an open gap condition with no pellet and clad contact occurring. For a closed gap condition, the expansion of the fuel pellet might also impose a mechanical stress on the cladding. Bending forces and creep deformation are ignored in the calculations.

C.3 Fuel and Clad Thermal Expansion

The temperature dependent fuel pellet thermal strain is used to calculate radial and axial thermal expansion for the fuel pellet. Radial thickness and axial height of the control volume are multiplied by the strain to calculate radial and axial thermal expansions. Axial average and radial volume average temperatures are used in the calculations. The total pellet expansion is determined by the summation of the thermal expansions of all control volumes in the pellet. For cladding radial thermal expansion, single control volume is used in the radial direction and clad mean radius is multiplied by the cladding strain in the calculation [1]. Axial thermal expansion of clad includes all axial nodes and use average cladding temperature at the given axial level.
C.4 Fuel Pellet Relocation

Fuel pellet geometry changes with a thermal expansion. In addition, the fuel pellet might also crack and causes it to creep further into the gap and even contact with the clad. The CTF use FRACAS-I mechanics relocation model incorporated cracking induced movement of the fuel pellet. The amount of pellet relocation in an open gap condition is described as a function of cold-state rod geometry [1].

\[(\Delta \text{rel})_{\text{fuel}} = \delta_0 - 0.005r_f\]  \hspace{1cm} (Equation C.1)

Where,

\(\delta_0\) denotes the as-fabricated fuel and clad gap size in ft,

\(r_f\) denotes cold-state radius of the fuel pellet in ft,

\(\Delta r\) denotes fuel pellet radius changes in ft.

In CTF dynamic gap conductance model, the closed gap condition is assumed when the gap thickness decreases to less than 3.6 times the sum of the clad and pellet surface roughness. Accordingly, model adjusts the size of the fuel relocation to be large enough to satisfy the gap closed while not causing mechanical expansion of the cladding.

C.5 Cladding Elastic Deformation

Cladding elastic deformation depends on the condition of the gap. If the gap is open, differential pressure between fill gas pressure and reactor system pressure will be the main reason for cladding stresses. On the other side, if the gap is determined to be closed, fuel pellet thermal expansion will become the dominant reason for the cladding stress. Both hoop stress and axial stress in the cladding are functions of the cladding inside and outside pressure. The radial deformation is calculated by multiplying the mean cladding radius by hoop strain and axial deformation is calculated by summing the axial expansion of each control volume in the axial direction. CTF theory manual provides detailed description of the model and calculations [1]
C.6 References


2. Geochemical Society Publications

   http://www.geochemsoc.org/publications/geochemicalnews/gn132jul07/disposalofnuclearwaste/
APPENDIX D

CTF PELLET-CLADDING DYNAMIC GAP CONDUCTANCE MODEL

D.1 CTF Pellet-Cladding Gap Conductance Model

The main goal of this research is to improve the fuel centerline prediction capabilities of CTF. It is very important to predict the fuel centerline temperatures accurately during steady state and accident conditions due to keeping it under the fuel material melting point to preserve fuel integrity. It was demonstrated in Chapter 3 that the two important parameters impacting most the fuel centerline temperatures were determined to be fuel thermal conductivity and gap conductance.

Fuel centerline temperature has a high sensitivity against a perturbation in fuel thermal conductivity parameter. However, gap conductance perturbations impact both fuel surface and centerline temperatures at the same magnitude. It was concluded that the gap conductance has a medium impact and has secondary importance in fuel centerline predictions with a greater impact on fuel average temperature predictions.

CTF Theory Manual [1] states that the dynamic gap conductance model has the following three sub components such as thermal radiation, conduction in the fill gas and conduction due to physical contact between the fuel pellet and the cladding. Gap is assumed axisymmetric in the calculations.

For IFA-681-r2 UO2/Gd2O3 fuel rod calculations performed by using the dynamic gap conductance model, it was observed that the dominant heat transfer mechanism in the gap is always conduction in the fill gas and its contribution in the total gap conductance value varies between 95-99 % of the total value, whereas, solid contact conductance term can change from 3 % up to 5 % depending on pellet-clad contact conditions in the gap. Typically, radiation component is less contributing factor with less than 0.1 %. Figure D-1 shows the components of the pellet-cladding gap conductance and their values for the IFA-681-r2 rod.
Figure D-1 Components of the Pellet-Cladding Gap Conductance for IFA-681-r2 rod

D.1.1 Radiant Heat Transfer

The gap conductance due to radiant heat transfer is expressed as the ratio of the gap radiant heat flux, $q_{r''}$, to the temperature rise across the fuel and cladding gap.

$$h_{rad} = \frac{q_{r''}}{T_f - T_c}$$  \hspace{1cm} \text{(Equation D.1)}

The radiant heat flux is calculated from the following Stefan-Boltzmann equation;

$$q_{r''} = \sigma_{SB} \frac{(T_f^4 - T_c^4)}{\varepsilon_f + \frac{\varepsilon_f}{A_f(1 - \varepsilon_f)}}$$  \hspace{1cm} \text{(Equation D.2)}

Where subscripts $f$ and $c$ stand for fuel and cladding, $\varepsilon$ denotes surface emissivity and $\sigma_{SB}$ refers to Stefan-Boltzmann constant ($1.714 \times 10^9$ BTU/hr-ft$^2$-R$^4$). Temperatures are provided in units of Rankine.
D.1.2 Conduction Heat Transfer in the Fill Gas

CTF [1] assumes that convection heat transfer caused by fill gas is negligible due to very thin gap structure between fuel rod and the cladding. Conduction heat transfer through the fill gas will exist whether the gap is open or closed due to fuel expansion, however, the calculation of heat conduction in the fill gas in a closed gap will be slightly different than that for that of open gap. CTF fuel deformation module calculates the physical gap thickness ($tg$) and the jump distances ($g_1$ and $g_2$) first. Then, CTF deformation module compares the physical gap thickness to combination of surface roughness of fuel and clad and dimensionless modification factor incorporating for interface pressure to determine whether the gap is closed or open. A gap is assumed to be closed when the calculated gap thickness is less than 3.6 times the sum of the surface roughness as shown in Equation D.3 below.

$$tg < 3.6 \times (R_1 + R_2)$$

(Equation D.3)

For both case, the gas heat conduction is defined as the gas mixture conductivity divided by the gap thickness.

$$H_{gas} = \frac{k_{gas}}{\delta_{gas}}$$

(Equation D.4)

Figure D.2 shows the temperature jump near the fuel pellet and clad surface based on incomplete thermal mixing of the gas molecules in the localized region.
CTF model incorporates the discontinuity while adding the temperature jump distances ($g_1$ and $g_2$) into the gas conduction equation given in Equation D.5. It is used for open gap calculation. The gas conductivity is given in units of BTU/hr-ft-ºF and the physical gap thickness, $t_g$, and jump distance units are in ft.

$$H_{gas} = \frac{k_{gas}}{t_g + (g_1 + g_2)}$$  \hspace{1cm} (Equation D.5)

After determining the existence of closed gap condition, CTF uses slightly different formula given in Equation D.6 for the calculation of gas fill gap conductance component. The model used for calculating gap fill heat conduction was based on a linear regression analysis of Ross-Stoudt data by Lanning and Hann [2].

$$H_{gas} = \frac{k_{gas}}{1.8 + C \cdot (R_1 + R_2) + (g_1 + g_2) - 4.2 \cdot 10^{-7}}$$  \hspace{1cm} (Equation D.6)
Where \( R_1 \) and \( R_2 \) represents surface roughness of fuel and clad in ft, dimensionless modification factor accounting for interface pressure, \( P_{\text{int}} \), is given as \( C \) and defined below:

\[
C = 1.98 \times \exp - 8.8 \times 10^{-5}P_{\text{int}}
\]

(Equation D.7)

Thermal conductivity of a mixture of gases is calculated by considering all the individuals gas conductivities and their molecular weights and fractions. In addition to thermal conductivity, temperature jump distance is also calculated based on Lloyd model [1]. The gas thermal conductivity and jump distance calculation model is described in CTF Theory Manual [1] in detail and it is not repeated here.

The gap temperature jump distance is given as a function of fill gas thermal conductivity, mean gas gap temperature, fill gas pressure and molecular fraction of each gas molecules in the gap.

### D.1.3 Pellet-Cladding Contact Conductance

The solid conduction term will be calculated when the deformation model determines that calculated gap thickness is small enough for a contact occur. Otherwise, the term will be assumed zero, if the contact condition is not met. The model is described here briefly and more information is available in the CTF theory manual [1]. The heat transfer coefficient calculation formula is given in Equation D.8 below.

\[
H_{\text{solid}} = \frac{5k_m}{\sqrt{R_f^2 + R_c^2}} \frac{(P_{\text{int}})}{H_Z} \left( \frac{R_f}{\lambda_f} \right)^n
\]

(Equation D.8)

Where

\( P_{\text{int}} \) = interface pressure;

\( H_Z \) = Meyer hardness of Zircaloy;

\( R_f \) and \( R_c \) = fuel and class roughness parameters in inches;

\( n\) = is based on the value of the non-dimensionalized interface pressure. For \( P_{\text{int}}/H_Z < 0.0001 \), \( n \) is set to 0.5. For values of \( P_{\text{int}}/H_Z \) between 0.001 and 0.01, the entire expression, \( (P_{\text{int}}/H_Z)^n \), is 0.01. For values of \( P_{\text{int}}/H_Z > 0.01 \), \( n \) is set to 1.0.

\( k_m \) = conductivity at the interface function of fuel and cladding conductivities:
\[ k_m = \frac{2k_fk_c}{k_f+k_c} \]  

(Equation D.9)

### D.2 Impact of Gap Conductance on Fuel Temperature Profile

IFA-681-r2 UO\textsubscript{2}/Gd\textsubscript{2}O\textsubscript{3} fuel rod was selected to show the impact of gap conductance model in the prediction of fuel centerline temperature and radial temperature profile. Fuel depletion step 17 was chosen with burnup value of 7.32 GWd/MTU. Halden experimental report [3] states that there is a pellet and clad contact and gap closure in this rod that makes it perfect candidate to analyze the impact of the gap conductance model. Figure D-3 shows the radial power profile used at this exposure in the fuel rod. CTF requires using equal radial mesh size due to radial nodal calculation schemes described in the CTF User Manual [1] in detail. Therefore, fuel performance code radial nodes used in the modeling of IFA-681-r2 during FRAPCON-3.4 calculations and radial power distribution (RPD) were converted to equal radial mesh size structure power profile shown in Figure D-3.

Figure D-4 demonstrates gap conductance profiles calculated by FRAPCON-3.4 versus CTF dynamic gap conductance model against rod axial height. The CTF dynamic gap conductance model estimates higher gap conductance values compared to FRAPCON-3.4 and it provides an axially uniform gap conductance.
Figure D-3 Radial Power Profile vs. Radial Node for IFA-681-r2 UO$_2$/Gd$_2$O$_3$

Figure D-4 Gap Conductance Profiles CTF Dynamic Gap vs. FRAPCON-3.4 for IFA-681-r2 UO$_2$/Gd$_2$O$_3$
D.3 Dynamic Gap Conductance Calculation

CTF dynamic gap conductance model predicts the gap conductance in the order of $10^5$ W/m²·ºK whereas FRAPCON predicts in the order of $10^4$ W/m². It results in a very small temperature increase in the gap compared to FRAPCON calculation. Figure D-5 shows the radial temperature profile comparison for CTF dynamic gap model versus FRAPCON calculation. FRAPCON calculates around 200ºF temperature jump in the gap due to low gap conductance value as compared to the CTF dynamic model. Therefore, fuel surface temperature differs for both calculations. CTF experience lower fuel surface temperature compared to FRAPCON temperature profile as expected. As a result, the CTF fuel thermal conductivity model determines higher fuel thermal conductivities near fuel surface in the fuel region due to lower fuel surface temperatures. This effect can be seen in Figure D-6 that shows radial thermal conductivity ($k_{th}$) profile comparison for CTF dynamic gap vs. FRAPCON. The differences in thermal conductivity profile are smaller towards near the center of the fuel rod as the fuel temperature profiles get closer to each other.

![Figure D-5 Radial Temperature Profile Comparison for CTF Dynamic Gap vs. FRAPCON](image)
D.4 Uniform Gap Conductance Calculation

The same calculation with the previous section was repeated by using uniform gap conductance value to understand the impact on the radial temperature profile and centerline temperature prediction. CTF and FRAPCON calculation both use the same gap conductance value of $10^4$ W/m²·ºK in this study. Figure D-7 shows radial temperature profile comparison for the calculation. The temperature jump in the gap matches the same value, which is around 200ºF. Radial fuel thermal conductivity profile is given in Figure D-8 and it starts with the same value at the fuel surface. Thermal conductivities exhibit differences towards to the center of the fuel rod and this results in a bigger centerline temperature difference and CTF over predicts the fuel centerline temperature around 250ºF as shown in Figure D-7 below.
Figure D-7 Radial Temperature Profile Comparison for CTF Constant Gap vs. FRAPCON

Figure D-8 Radial Thermal Conductivity Profile Comparison for CTF Constant Gap vs. FRAPCON
D.5 Comparison and Conclusions

As a conclusion from this sensitivity study, the dynamic gap conductance model is the recommended option to be used in the calculations, if there is fuel and clad closure and contact for the specified fuel rods instead of using fuel performance code predicted uniform gap conductance value in the coupling or code-to-code comparison calculations. Otherwise, the centerline temperature will over predict the expected results due to impact of gap closure (See Figure D-9). The dynamic gap conductance model was developed long time ago based on experimental data regression analysis of Ross-Stoudt data by Lanning and Hann [2] and gap conductance parameter was determined to fit the measured experimental temperature drop data across the gap for different conditions. Therefore, the CTF predicted temperature drop across the fuel gap will be different compared to fuel performance code predictions due to modification and adjustment to gap conductance value. However, it will provide more conservative fuel centerline temperature predictions. Therefore, the dynamic gap conductance model should be recommended for coupled thermal hydraulic and fuel performance code calculations. To demonstrate this behavior, Figure D-9 shows the radial temperature profiles comparison for CTF dynamic and constant gap models versus FRAPCON.
Figure D-9 Radial Temperature Profiles Comparison for CTF Dynamic and Constant Gap vs. FRAPCON
D.6 References


APPENDIX E

IMPACT OF RADIAL NODAL/AVERAGE THERMAL CONDUCTIVITY
ON FUEL TEMPERATURE PROFILE

This section discusses the impact of using radial nodal versus radial average thermal conductivity in a sample PWR single fuel rod radial temperature profile calculation. Figure E-1 demonstrates the radial fuel nodes and rings used for a single fuel rod temperature profile calculations. There are total seven radial fuel nodes available in the model.

![Figure E-1](image)

Analytical Solution for a solid cylindrical fuel rod temperature profile is given below [1]:

\[
\int_T^{T_{\text{max}}} \frac{kdT}{r^2} = q''' \frac{r^2}{4}.
\]  

(Equation E.1)

As an example, temperature of node 6 of the above model can be calculated by using radial nodal thermal conductivities:

\[
K_6 T_6 - K_7 T_7 = q''' \frac{(R_6^2 - R_7^2)}/4.
\]  

(Equation E.2)

The temperature becomes:

\[
T_6 - K_7 T_7 / K_6 = q''' \frac{(R_6^2 - R_7^2)}/4K_6.
\]  

(Equation E.3)
On the other hand, if we use average thermal conductivity in all radial nodes \((K_7=K_6=K_{\text{average}})\), the temperature becomes:

\[ T_6 - T_7 + q''' \left( R_6^2 - R_7^2 \right)/4K_{\text{average}}. \]  

(Equation E.4)

Similar equations are used for all fuel nodes temperature calculations. Figure E-2 shows the difference of average versus radial thermal conductivities at each radial nodal ring of the fuel rod. Radial nodal thermal conductivity reduces going toward the center of the fuel rod near 1 due to calculated high temperature near the center of fuel rod. If the average thermal conductivity is preferred to be used in the calculations, the maximum thermal conductivity difference is observed at the surface of the rod and node 7, and it is 0.6 W-m/°K. The use of an average thermal conductivity underestimates the calculation between node 5 and node 7. However, it overestimates the thermal conductivity near the center of fuel rod due to the higher temperature and the maximum difference is -0.3 W-m/°K at node 1. Figure E-3 shows the comparison of radial nodal temperature profiles for nodal versus average thermal conductivities. Both calculations demonstrate that the second order polynomial profile making peak at the center of the solid cylindrical fuel rod. The temperature profiles difference has an increasing trend towards the center node 1. The maximum temperature difference is observed at the center node 1 and it is around 163°K for a typical PWR single fuel rod and the use of average thermal conductivity underpredicts the temperature estimation. This shows the importance of using radial nodal ring thermal conductivity models in estimating the temperature profile of fuel rods versus assuming average thermal conductivity in a single fuel rod.
**Figure E-2** Comparison of Radial Nodal vs. Radial Average Thermal Conductivities

**Figure E-3** Comparison of Radial Temperature Profiles for Nodal vs. Average Thermal Conductivities
E.1 References

APPENDIX F

CTF SINGLE CHANNEL SAMPLE INPUT DECK

*******************************************************************************
* CTF input for a High-Burnup MOX single-pin case from Purdue MOX benchmark *
* Model 3: CTF/TORT-TD
*******************************************************************************

--- Card 0.1 -----------------------------------------------------------------
* ICOBRA
  1

--- Card 0.2 -----------------------------------------------------------------
* INITIAL DUMPF
  1 0

--- Card 0.3 -----------------------------------------------------------------
* EPSO OITMAX IITMAX COURANT
  0.001 10 40 0.8

--- Simulation ID -------------------------------------------------------------
*** Pin-Test ***

*******************************************************************************
* CARD GROUP 1: Selection of the Physical Models, Global Boundary Conditions,
* and Initial Conditions
*******************************************************************************

*NGRP
1

--- Card 1.1 -----------------------------------------------------------------
*NGAS IRFC EMED IMIX ISOL GINIT NTRN MESH IFRAP ND10 ND11 ND12 ND13 ND14
  1 2 1 1 0 0.0 0 1 1 0 0 0 0 0

--- Card 1.2 -----------------------------------------------------------------
*GTOT AFLUX OIFRAC
  0.284157 23.13 0.0

--- Card 1.3 -----------------------------------------------------------------
*PREF HIN HGIN VFRAC1 VFRAC2
  155. 1268. 300.0 1.0 0.9999

--- Card 1.4 -----------------------------------------------------------------
*GTYPE VFRAC
**CARD GROUP 2: Channel Description**

*NGRP 2

--- Card 2.1

*NCHANL ND02 ND03 ND04 ND05 ND06 ND07 ND08 ND09 ND10 ND11 ND12 ND13 ND14
1 0 0 0 0 0 0 0 0 0 0 0 0 0

--- Card 2.2

*I AN PW ABOT ATOP NAMGAP X Y XSIZ YSIZ
1 0.000928 0.0288 0.0 0.0 0 2 2 0.0126 0.0126

**CARD GROUP 4: Vertical Channel Connection Data**

*NGRP 4

--- Card 4.1

*NSECTS NSIM IREBAL ND04 ND05 ND06 ND07 ND08 ND09 ND10 ND11 ND12 ND13 ND14
1 1 0 0 0 0 0 0 0 0 0 0 0 0

--- Card 4.2

* Active length

*ISEC NCHN NONODE DXS IVARDX
1 1 20 0.18288 0

--- Card 4.4

*I KCHANA x 6 KCHANB x 6
1 1 0 0 0 0 1 0 0 0 0 0

--- Card 4.5

*INIDE
1

--- Card 4.6

*MSIM
20

--- Card 7.1

*NCD NGT IFGQF IFSDRP IFESPV IFTPE IGTEMP NFBS ND09 ND10 ND11 ND12 ND13 ND14
10 0 0 0 0 0 0 0 0 0 0 0 0 0
*--- Card 7.2 -----------------------------------------------------------------
*CDL     J IC01 IC02 IC03 IC04 IC05 IC06 IC07 IC08 IC09 IC10 IC11 IC12
1.7001  2 1    0    0    0    0    0    0    0    0    0    0    0
1.7001  4 1    0    0    0    0    0    0    0    0    0    0    0
1.7001  6 1    0    0    0    0    0    0    0    0    0    0    0
1.7001  8 1    0    0    0    0    0    0    0    0    0    0    0
1.7001 10 1    0    0    0    0    0    0    0    0    0    0    0
1.7001 12 1    0    0    0    0    0    0    0    0    0    0    0
1.7001 14 1    0    0    0    0    0    0    0    0    0    0    0
1.7001 16 1    0    0    0    0    0    0    0    0    0    0    0
1.7001 18 1    0    0    0    0    0    0    0    0    0    0    0
1.7001 20 1    0    0    0    0    0    0    0    0    0    0    0
********************************************************************************
* CARD GROUP 8: Rod and Unheated Conductor Data
*******************************************************************************
*--- Card 8.1 -----------------------------------------------------------------
*NGRP
8
*--- Cards 8.2 & 8.3 ----------------------------------------------------------
*N IFTYP IAXP NRENODE DAXMIN RMULT HGAP ISECR HTAMB TAMB
1 1     1    0       0.     1.   100000.   1     0.    0.
*NC PIE NC PIE NC PIE NC PIE NC PIE NC PIE NC PIE NC PIE
1 1.0  0  0.0  0  0.0  0  0.0  0  0.0
*--- Card 8.6 -----------------------------------------------------------------
*I NRT1 NST1 NRAX1
1 1    0    2
*--- Card 8.7 -----------------------------------------------------------------
*IRTAB
1
*--- Card 8.9 -----------------------------------------------------------------
*AXIAL TRINIT
0.300.
3.6576 300.
*Card 8.13
*Fuel Rod Index
1
*EXPOSURE GADCON IMOX
35.0  0.0  1
35.0  0.0  1
35.0  0.0  1
35.0  0.0  1
* CARD GROUP 9: Conductor Geometry Description
*******************************************************************************
*NGRP
9
**** High-burnup MOX ****
*IFTYPE DROD   DFUEL   NFUEL  IMATF  IMATC  IMATOX  DCORE  TCLAD  FTDENS  IGFC  IGFORC  IRADP
1  nucl  0.009166  0.007902  15    0     0     0      0     0.000573  0.9471    0   0      17
*PGAS  VPLEN    ROUFF  ROUFC  GSFRAC(1..6)    OXIDET
25.8  1.1114e-5  2.0e-6  5.0e-7  1.  0.  0.  0.  0.  0.  0.
*AXJ    AGFACT
3.6576  1.82525e-05
*RADP  POWR
0.0588  0.7767
0.1176  0.7803
0.1765  0.7821
0.2353  0.7857
0.2941  0.7876
0.3529  0.7938
0.4118  0.8000
0.4706  0.8066
0.5294  0.8171
231

* CARD GROUP 11: Axial Power Distribution Tables, Radial Power Distributions, 
* and Transient Forcing Functions
*******************************************************************************
* NGRP
   11
*--- Card 11.1 -----------------------------------------------
*NGQA NAXP MNXN NQ NGPFF NQR ND07 ND08 ND09 ND10 ND11 ND12 ND13 ND14
 1 1 22 0 0 1 0 0 0 0 0 0 0 0
*--- Card 11.2 -----------------------------------------------
*YQA
  0.
*--- Card 11.3 -----------------------------------------------
*I NAXN
  1 22
*--- Card 11.4 -----------------------------------------------
*Y AXIALZ
  0.00000  0.180682098
  0.09144  0.323781568
  0.27432  0.609980506
  0.4572  0.858598817
  0.64008  1.060964049
  0.82296  1.211290562
 1.00584  1.321147632
 1.18872  1.38473961
 1.3716  1.41943424
 1.55448  1.428101873
 1.73736  1.410764976
 1.92024  1.370285523
 2.10312  1.315361993
 2.286  1.243091556
 2.46888  1.147688573
 2.65176  1.040724322
 2.83464  0.91352535
 3.01752  0.763198837
 3.2004  0.598417236
 3.38328  0.416289729
 3.56616  0.222599953
3.6576 0.125755065
*
*** Card 11.7 -------------------------------------------------------------
*YQR 0.
*
*** Card 11.8 -------------------------------------------------------------
*FQR 1.
*
******************************************************************************
* CARD GROUP 12: Turbulent Mixing and Void Drift Data
******************************************************************************
*
*NGRP 12
*** Card 12.1 -------------------------------------------------------------
*AAAK BETA 1.4 0.004
*
******************************************************************************
* CARD GROUP 13: Boundary Condition Data
******************************************************************************
*
*NGRP 13
*** Card 13.1 -------------------------------------------------------------
*NBND NKBD NFUN NGBD NDM5 NDM6 NDM7 NDM8 NDM9 NM10 NM11 NM12 NM13 NM14
2 0 1 0 0 0 0 0 0 0 0 0 0 0
*
*** Card 13.2 -------------------------------------------------------------
*NPTS 3
*
*** Card 13.3 -------------------------------------------------------------
*ABSC ORDINT ABSC ORDINT ABSC ORDINT
0.0 0.0 0.1 1.0 1.0e6 1.0
*
*** Card 13.4 -------------------------------------------------------------
* Inlet b.c.
*IBD1 IBD2 ISPC N1FN N2FN N3FN BCVALUE1 BCVALUE2 BCVALUE3 INITGAS
1 1 2 1 0 0 0 1267.9 0. 1
* Outlet b.c.
*IBD1 IBD2 ISPC N1FN N2FN N3FN BCVALUE1 BCVALUE2 BCVALUE3 INITGAS
1 22 1 0 0 0 0. 1267.9 155. 1
*
******************************************************************************
* CARD GROUP 14: Output Options
******************************************************************************
*
*NGRP
*--- Card 14.1 ---------------------------------------------------------------
*   N1 NOU1 NOU2 NOU3 NOU4 IPRP IOPT NDM8 NDM9 NM10 NM11 NM12 NM13 NM14
5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
* *******************************************************************************
* CARD GROUP 16: TORT Coupling Description  
* *******************************************************************************
* NGRP
16
*--- Card 16.1 ---------------------------------------------------------------
* NMAPS NX NY NZ DZBR DZTR DT
1 1 1 24 0.3 0.3 -1.0
*  
*--- Card 16.2 ---------------------------------------------------------------
* AERR MERR AVIT MXIT
0.00001 0.0001 0 100
*  
*--- Card 16.3 ---------------------------------------------------------------
* IMXY
1
*  
*--- Card 16.4, 16.5, & 16.6 --------------------------------------------------
* INCH RTYP IROD NAZIM
* CHWT
* ICHAN
* row 1
1 1 1 1
1.0
1
*  
* *******************************************************************************
* CARD GROUP 30: Time Domain Data  
* *******************************************************************************
* NGRP
30
*--- Card 30.1 ---------------------------------------------------------------
* DTMIN DTMAX TEND EDINT DMPINT RTWFP
0.00001 0.01 1.0e6 1.0e6 0. 1.
0.00001 0.01 1.0 0.1 0.0 1.0
* DTMIN (if negative stop)
-1.0 0. 0. 0. 0. 0.
APPENDIX G

CODE UNCERTAINTIES

The Nuclear Energy Agency of the Organization for Economic Co-operation and Development (NEA/OECD) sponsored benchmark study for uncertainty analysis in modelling design, operation and safety analysis of LWRs [1], which provided detailed information regarding fuel performance codes and bundle thermal hydraulics codes uncertainties. This appendix summarizes the information as follows. Section G.1 describes the FRAPCON/FRAPTRAN code uncertainties and Section G.2 describes the CTF code uncertainties.

G.1 Fuel Performance Code Uncertainties

G.1.1 Input Uncertainties

The input uncertainty parameters, which are defined with upper and lower bounds and a distribution type, are grouped by source below:

a) Uncertainties in manufacturing tolerances:

- Cladding outside/inside diameter,
- Cladding thickness,
- Cladding roughness,
- Fuel pellet outside diameter,
- Fuel pellet roughness,
- Fuel density,
- Gap fill pressure,
- Fuel enrichment.
b) Uncertainties in boundary conditions:

- System pressure,
- System power,
- Coolant inlet temperature,
- Coolant flow rate.

The boundary condition uncertainties in terms of upper and lower bounds, as well as the type of distribution are provided in Table G-1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>BWR</th>
<th>PWR</th>
<th>VVER</th>
<th>Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>System pressure (%)</td>
<td>± 1.0</td>
<td>± 1.0</td>
<td>± 2.0</td>
<td>Normal</td>
</tr>
<tr>
<td>Coolant flow rate (%)</td>
<td>± 5.0</td>
<td>± 5.0</td>
<td>± 5.0</td>
<td>Normal</td>
</tr>
<tr>
<td>System power (%)</td>
<td>± 5.0</td>
<td>± 5.0</td>
<td>± 5.0</td>
<td>Normal</td>
</tr>
<tr>
<td>Inlet fluid temperature (K)</td>
<td>± 3.0</td>
<td>± 3.0</td>
<td>± 3.0</td>
<td>Uniform</td>
</tr>
</tbody>
</table>

**G.1.2 Output Uncertainties**

The output uncertainties are:

- Fuel temperature,
- Fission gas release,
- Fuel cladding creep,
- Axial elongation,
- Fuel thermal expansion,
- Cladding thermal conductivity,
- Cladding thermal expansion.
G.2 Bundle Thermal Hydraulics Code Uncertainties

G.2.1 Input Uncertainties

The input uncertainties are grouped into the following categories:

a) Boundary condition uncertainties:
   - Pressure,
   - Coolant flow rate,
   - System power,
   - Inlet coolant temperature,
   - Uncertainties in the power distribution.

b) Geometry uncertainties:
   - Rod displacement,
   - Rod outer diameter.

The boundary conditions are shown in Table G-2 along with their distributions. The bounds are defined as three standard deviations. The manufacturing uncertainties are also shown in Table G-3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>BWR</th>
<th>PWR</th>
<th>VVER</th>
<th>Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>System pressure (%)</td>
<td>± 1.0</td>
<td>± 1.0</td>
<td>± 2.0</td>
<td>Normal</td>
</tr>
<tr>
<td>Flow rate (%)</td>
<td>± 1.5</td>
<td>± 1.0</td>
<td>± 4.5</td>
<td>Normal</td>
</tr>
<tr>
<td>Power (%)</td>
<td>± 1.0</td>
<td>± 1.5</td>
<td>± 0.3</td>
<td>Normal</td>
</tr>
<tr>
<td>Inlet fluid temperature (K)</td>
<td>± 1.5</td>
<td>± 1.0</td>
<td>± 2.0</td>
<td>Uniform</td>
</tr>
<tr>
<td>Power distribution (%)</td>
<td>± 3.0</td>
<td>± 3.0</td>
<td>± 3.0</td>
<td>Normal</td>
</tr>
</tbody>
</table>

Table G-3 Geometry Variations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>BWR</th>
<th>PWR</th>
<th>VVER</th>
<th>PDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rod displacement (mm)</td>
<td>± 0.45</td>
<td>± 0.45</td>
<td>± 0.45</td>
<td>Normal</td>
</tr>
<tr>
<td>Rod diameter (mm)</td>
<td>± 0.04</td>
<td>± 0.02</td>
<td>± 0.10</td>
<td>Normal</td>
</tr>
</tbody>
</table>
G.2.2 Output Uncertainties

The output uncertainties are:

- Maximum cladding temperature;
- Maximum fluid temperature;
- Maximum void fraction;
- Onset of nucleate boiling;
- Margin to Critical Heat Flux (Departure from Nucleate Boiling Ratio or Critical Power Ratio);
- Cladding temperature of the corner rod;
- Fluid temperature or void fraction of each subchannel surrounding the corner rod;
- Pressure drop.

G.3 References

VITA

Mine Ozdemir Yilmaz was born on August 23, 1979 in Ankara, Turkey. She received her B.S. in Petroleum and Natural Gas Engineering from Middle East Technical University, Ankara, Turkey in 2002. Afterwards, she started graduate school at Penn State University, University Park, PA and got her M.S. in Petroleum and Natural Gas Engineering in 2004. During her graduate study, she was a research assistant and worked on a DOE sponsored project called “Sonication”. She conducted experimental studies and investigated the effect of ultrasonic radiation on rock permeability.

She started to work for GE-Hitachi Nuclear Energy in 2006 as a computational thermal-hydraulics methods engineer and has been working for Methods & Software Development Group since then. She has been working on thermal-hydraulics methods code development, verification/validation, maintenance of nuclear engineering codes and methods required for BWR steady-state and transient analysis. She obtained her M.Eng. in Nuclear Engineering in 2010 and her Ph.D. in Nuclear Engineering in December 2014 both from Penn State University.

She lives in Wilmington, NC with her beloved husband Serkan Yilmaz and her two kids, twins, Serra and Kenan Arda who were born in August 2012. Her research area includes bundle thermal hydraulics, two phase flow, heat transfer, methods/code development and nuclear fuel performance.