ATOMISTICALLY INFORMED FUEL PERFORMANCE CODES: A PROOF OF PRINCIPLE USING MOLECULAR DYNAMICS AND FRAPCON SIMULATION

By

DANIEL ARMANDO VEGA

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To Sandwich, my patient cohort

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LIST OF ABBREVIATIONS AND TERMS

BOL	Beginning of life: freshly fabricated fuel, zero burnup.
Burnup	A pseudo-intensive property describing the amount thermal energy released per unit mass of nuclear fuel. Typically given in units of megawatt days per kilogram of Uranium (MWd/kg U)
CRUD	Chalk river unidentified deposits: corrosion and wear products (rust particles, etc.) that become radioactive (i.e., activated) when exposed to radiation.
EOL	End of life: time/burnup level associated with the end of a fuel rod's lifetime, at which point it is removed from the core and becomes spent fuel
LWR	Light water reactor: a thermal nuclear reactor that uses ordinary water (light water) as both its neutron moderator and coolant. Typically, either Pressurized Water Reactors (PWRs) or Boiling Water Reactors (BWRs).
MD	Molecular dynamics
Phonon	A quantized lattice vibration, modeled as a means for heat transfer in a rigid lattice
Polaron	A quasi-particle composed of an electron plus its accompanying polarization field. At high temperatures, becomes significant in heat transfer
PWR	Pressurized Water Reactor: a nuclear reactor that uses a pressure vessel around the core, keeping it under high pressure to prevent water in the primary cooling loop from boiling. Most reactor worldwide are PWRs.
IMF	Inert matrix fuel

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Daniel Armando Vega

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Current limitations on Uranium dioxide fuel lifetime are determined largely from physical degradation of the fuel pellets. In order to better understand the behavior of Uranium dioxide fuel, new atomic level approaches are being used to simulate the effects of both temperature and burnup. A proof-of-principle study is presented in which the results of atomic-level simulations of the thermal expansion and thermal conductivity of Uranium dioxide are integrated into the Light Water Reactor fuel performance code FRAPCON. The beginning of life (BOL) thermal conductivity profile of a fuel pellet, and the evolution of the pellet expansion over its lifetime are calculated. It is found that (i) modifying FRAPCON in such a way as to accept input from the results obtained through atomistic simulations by the integration of atomistic models into FRAPCON is possible for a number of thermo-mechanical properties, and (ii) the properties determined from atomistic simulations yield predictions in FRAPCON that are in good agreement for the BOL thermal conductivity, but less satisfactory for the pellet thermal expansion, due to phenomena thus far unaccounted for by atomic level simulations. Still, by successfully incorporating these simulations into FRAPCON, a basis for a more complete atomistic model is built, demonstrating the potential for more sophisticated and encompassing first principles models.

CHAPTER 1
INTRODUCTION

Having been in operation for over 35 years, LWRs using uranium dioxide (UO_2) fuel have been modeled and studied using a variety of neutronic, thermo-hydraulic, and thermo-mechanical approaches. Traditionally, the development of such simulations has been guided by studying the macroscopic phenomena characterized in laboratory experiments and during commercial reactor operations. A key part of the development and qualification of UO_2 fuel systems consists of analysis in fuel performance codes such as FRAPCON.[1] FRAPCON-3, the most recent release, encapsulates the behavior of UO_2 fuel pellets in terms of specific thermo-mechanical phenomena and carefully determined and validated empirical relationships. This approach has been extraordinarily successful in providing quantification of fuel properties. However, the development of the key empirical relationships is extremely time-consuming and expensive.

In addition, such empirical relationships are often valid only for discrete cases, creating simulations with proprietary modules; thus, any approaches that could reduce the time and expense involved while extending the scope of validity of the models would be extremely valuable. In this investigation, the first steps in using results from atomistic models, specifically molecular-dynamics simulations, directly as models into FRAPCON-3, is explored. The first step in this investigation is to study the nature and structure of FRAPCON-3 to determine the most prudent sections of source code to modify for atomistic simulation. Secondly, an appropriate description of the Atomistic/Molecular Dynamics Model (AM/MD) is presented. Then, a discussion of the coupled simulation methodology is presented, in which the integration of the FRAPCON and AM/MD is explained. Finally, the results obtained by this coupled simulation are presented for analysis and recommendations.

It is important to note that while atomic-level simulation can be powerful, the modeling of every component of a nuclear core is substantial and outside the scope of this investigation; thus atomic level simulation for this project pertains only to the UO_2 fuel pellets, keeping the thermal transport of the gap, cladding, and coolant unchanged. In addition, the fuel rod-specific macroscopic parameters by which fuel performance is based, is composed of a complex set of relationships describing geometry-dependent phenomena, material region interfaces, and composition changes. At this point in the AM/MD model, many of these phenomena have not yet been described. However, the most fundamental aspects of thermo-mechanical properties modeling, namely the thermal conductivity and thermal expansion, are appropriate candidates for rigorous first-principles modeling. By first establishing and validating these radically different models by comparing them to established models, the avenue for first principles investigations of yet to be modeled fuel lattices becomes widened. Such a bridge from empirical to first-principles models is a theme central to this investigation.

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CHAPTER 2
FRAPCON-3 FUEL PERFORMANCE CODE

2.1 FRAPCON Objectives

Fundamentally, the FRAPCON series was created to accurately calculate the performance of LWR fuel rods[3]: a major objective of the reactor safety research program sponsored by the U.S. Nuclear Regulatory Commission (NRC). As a result of an extensive analytical performance code development program, FRAPCON was created as a joint effort between Idaho National Engineering and Environmental Laboratory (INEEL) and Pacific Northwest National Laboratory (PNNL). INEEL has since become Idaho National Laboratory (INL), and both facilities are now operated by Battelle. With the creation of such a code, the NRC has the ability to not only achieve the object of accurately calculating thermo-mechanical properties and performance of fuel rods, but to independently investigate design parameters put forth by both nuclear vendors and utilities without using proprietary performance codes. By using both in-reactor and out-of-reactor experiments to benchmark and asses the code capabilities, FRAPCON has proven to be a reliable tool for simple analysis of LWR fuel rod performance. It is important to note that FRAPCON is a "steady state" code, which refers to the situation where (i) short-term changes are sufficiently small that they can be considered constant for a discreet time step, and (ii) boundary conditions for each iteration do not change. This analysis is valid for constant power and slow up-ramp or down-ramp operations typical of normal commercial reactor operations. Reactor accidents and transient analysis are included in FRAPTRAN, and not discussed in this investigation.

2.2 FRAPCON-3 Solution Description

In order to evaluate steady state fuel rod performance, FRAPCON-3 uses an iterative process based on defined boundary conditions at each time step. Simply put, the interrelated

effects of fission rate, thermal energy distribution, fuel and cladding temperature, fission product release, fuel swelling/densification, irradiation-induced growth, thermal expansion, crud deposition, cladding corrosion are coupled together and run through calculation loops until temperature solutions converge to within an acceptable error range. Naturally, some of these phenomena are fuel rod power/temperature specific, while others are cumulative, and heavily dependent on burnup and previous conditions. For this reason, a collection of loops is used to calculate the properties for each time step. Because the number and length of time steps is user defined, it is apparent that increased accuracy can be achieved with finer time steps, while computational demand can be assuaged by more coarse time steps. Much of the information in this section is adapted from the FRAPCON manual,[3] and the components most pertinent to this investigation are included in this section. At the beginning of each time step, a number of operations are carried out:

1. Initial fuel rod data is determined by input from previous step (or initial condition)
2. Temperature of fuel and cladding are computed
3. Fission product generation & release, internal gas pressure computed
4. Temperature response is iterated through loop until solution converges to less than 1% of ΔT

When the temperature converges, the parameters are all recorded, sent to the output file, and used for the initial conditions for the next time step. Figure 2-1 gives a simplified solution scheme flow chart.

2.3 Fuel Rod Thermal Conductivity Response Calculation

To further simplify heat transport calculations, each calculation for the fuel pellet temperature distribution is taken in such a way that heat transfer is only in the radial direction. This is a valid assumption if one assumes (i) azimuthal homogeneity (axissymmetric analysis),

and (ii) for each axial node, heat transfer in the axial direction is negligible as compared to that in the radial direction, and is thus ignored (Figure 2-2).

The centerline temperature of the pellet, being the innermost and hottest component, is the first temperature calculated, followed by the pellet surface temperature, the inner cladding temperature, the outer cladding temperature, the oxidation layer temperature, and finally, the bulk coolant temperature. In simple terms, the temperature change from the fuel centerline to the bulk coolant can be given in terms of component temperature changes by the equation:

$$T_{fc}(z) = T_{bulk}(z) + \Delta T_{film}(z) + \Delta T_{crud}(z) + \Delta T_{ox}(z) + \Delta T_{clad}(z) + \Delta T_{gap}(z) + \Delta T_{fuel}(z) \quad \textbf{(1-1)}$$

where

T_{fc} = fuel centerline temperature

T_{bulk} = bulk coolant temperature

ΔT_{film} = temperature change through the forced convection film layer

ΔT_{crud} = temperature change through crud layer

ΔT_{ox} = temperature change through oxide Layer

ΔT_{clad} = temperature change through cladding

ΔT_{gap} = temperature change through gap

ΔT_{fuel} = temperature change through fuel pellet

2.3.1 Fuel Pellet Thermal Energy Distribution and Conduction Model

While conduction through each region is important, for the purposes of this section, only the conduction through the pellet is analyzed. This is because the pellet is the only region to which fundamental source code changes are made for the FRAPCON-AM/MD investigation.

The finite difference (FD) heat conduction models used on FRAPCON-3 are based on those presented in RELAP-5.[4] Instead of the method of weighted residuals used in previous releases of FRAPCON, the FD approach used in FRAPCON-3 must contain fine-mesh capabilities for high burnup analysis, and must interface with other burnup models – either in existence or yet to be created.[3]

While an FD approach is straightforward for localized or uniform heat sources, the non-uniformity of internal energy production requires that the FD method take into account the spatial dependence of internal heat sources. In addition, because FRAPCON-3 contains a user-defined number of temperature nodes, as well as variable mesh spacing, the FD method must allow for such flexibility. The steady-state integral form of the heat conduction equation is:

$$\iint_S k(T,\bar{x})\vec{\nabla}T(\bar{x}) \bullet \vec{n}\partial s = \iiint_V S(\bar{x})\partial V \qquad \textbf{(1-2)}$$

Where

k = thermal conductivity (W/m-K)

s = surface of control volume (m^2)

$\vec{n}$ = surface normal unit vector

S = internal heat source (W/m^3)

T = temperature (K)

V = control volume (m^3)

$\bar{x}$ = 1-D space coordinate

It is apparent that Equation 1-2 is complex enough in 1-D that thousands of FD calculations require a fair amount of computation. 2-D and 3-D models of this variety would require far greater computation resources. Figure 2-4 shows the 1-D mesh point layout. In order to maintain proper control surface and volume integrals, it is an important assumption that the geometry remains fixed for this stage in the analysis. In addition, boundary conditions must be established. For all FD calculations in the fuel pellet, the following boundary conditions are used:

1) $\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0$ (pellet center is local maximum, azimuthal symetry)

2) Pellet Surface Temperature (T_{fs}) is defined

Once a suitable temperature distribution is established, FRAPCON-3 can exit the fuel pellet temperature subroutine and continue with gap, cladding, oxide, crud, and bulk temperature calculations. When a distribution has been established for the entire rod, the thermal expansion and stress/strain relationships expressed in other subroutines can be evaluated within the same coarse time step.

In words, equation 1-2 states that for a steady state fuel pellet, the integrated surface heat flux through the control area into the gap (left hand side) is equal to the integrated heat generation rate in the control volume (right hand side). With this in mind, the numerical solutions to this equation are based on correct balance of temperature and conductivity, equivalent to a heat generation rate. When incorporating an AM/MD model, there is no reason to re-evaluate the FD methodology. In fact, in order to discover how the materials properties affect the overall performance of the fuel rod, it is important to maintain code structure for the fuel pellet temperature distribution. Returning to equation 1-2, the only parameter that should change is the thermal conductivity $k(T,\overline{x})$ function. In order to understand where this term comes from, as well as how it compares to an AM/MD model, the following section presents a description of the thermal conductivity function.

2.3.2 FRAPCON Thermal Conductivity Function

In general, and in the context of FRAPCON, thermal conductivity (k) has a dependence on temperature. The thermal conductivity function chosen as a base case for use throughout this investigation is and currently used in FRAPCON-3.3 is one presented by staff at Nuclear Fuel Industries, Ltd. (Japan), at the May1997 American Nuclear Society Topical meeting on Light Water Reactor Fuel Performance.[5] The NFI function is of the same form as that originally included in FRAPCON-3 by Lucata et al.[6] Equations 1-3 and 1-4 represent these functions,

respectively. While the functions are similar, the NFI function was chosen, because it is included in the most recent FRAPCON-3 release (FRAPCON-3.3). This function has been successfully benchmarked, and provides a better fit to collected data from a study by Ronchi.[8] The study provides a suitable base for typical PWR fuel conductivity calculations:

$$k_o = \frac{1.0}{(0.0452+0.000246\times T)} + \left(\frac{3.50\times 10^9}{T^2}\right)e^{\left(\frac{-16361}{T}\right)} \qquad \textbf{NFI} \qquad \textbf{(1-3)}$$

$$k_o = \frac{1.0}{(0.0375+0.0002165\times T)} + \left(\frac{4.715\times 10^9}{T^2}\right)e^{\left(\frac{-16361}{T}\right)} \qquad \textbf{Lucata} \qquad \textbf{(1-4)}$$

where

k_o = conductivity of unirradiated urania (UO_2)

T = temperature (K)

The gadolinia content for this fuel pellet is 0. The conductivity of unirradiated 95% dense (theoretical) urania thus becomes the starting point for burnup calculations. Figure 2-5[7] gives a plot of the NFI function, Lucuta function, and experimental data, collected by Ronchi, et al, 1999.[8] The Ronchi (1999) data come from a study done on unirradiated pellet material at nominal and high temperatures. A final function describing the conductivity used for calculation throughout the time step is given by multiplying k_o by a collection of four coefficients representing particular burnup and non-burnup phenomena. These coefficients are:

FD - dissolved fission product (temperature and burnup dependent)

FP - precipitated fission product (temperature and burnup dependent)

FM - Maxwell porosity factor (porosity fraction and shape factor)

FR - radiation effect (temperature dependent)

FD becomes an increasingly significant coefficient as temperature and burnup increase, as is evident in its definition:

$$FD = \frac{1.09}{B^{3.265}} + \frac{0.0643}{\sqrt{B}}\sqrt{T}\arctan\left[\frac{1}{\frac{1.09}{B^{3.265}} + \frac{0.0643}{\sqrt{B}}\sqrt{T}}\right] \quad \textbf{(1-5)}$$

where

B = burnup (atom %) – 1 atom% = 9.383 GWd/MTU at 200 MeV/fission

T = temperature (K)

FP also increases with burnup and temperature, and is given by:

$$FP = 1 + \left[\frac{0.019B}{3 - 0.019B}\right]\left[\frac{1}{1 + e^{\left(\frac{1200-T}{100}\right)}}\right] \quad \textbf{(1-6)}$$

FM, which is related only to porosity, is given by:

$$FM = \frac{1-p}{1+(s-1)p} \quad \textbf{(1-7)}$$

where

p = porosity fraction (as fabricated plus swelling)

s = shape factor (1.5 for spheres)

FR, which is temperature-dependent and always applied, is given by:

$$FR = 1 - \left[\frac{0.2}{1 + e^{\left(\frac{T-900}{80}\right)}}\right] \quad \textbf{(1-8)}$$

Finally, these coefficients are put together and multiplied by k_o to give a temperature-burnup dependent thermal conductivity value (Equation 1-9) and the FD interval of interest is used for the corresponding temperature, to create a straightforward calculation for instantaneous thermal conductivity of the fuel pellet:

$$k = k_o(FD \times FP \times FM \times FR) \quad \textbf{(1-9)}$$

This calculation is then carried out for each radial node, after which other FD calculations are performed for the gap, cladding, oxide, and film layers. The thermal distributions for non-fuel regions will not be discussed in this investigation.

2.4 Fuel Rod Thermal Expansion and Mechanical Response

Thermal expansion is important to study because its effects lead to structural stress and corresponding phenomena, as well as changing the thermal conductivity coefficient. In addition, proper modeling of thermal expansion is necessary to accurately model other geometry-dependent phenomena, such as fission gas release.

FRAPCON-3 uses the FRACAS-I[9] mechanical model to calculate the fuel and cladding mechanical deformation throughout reactor operation. It is important to note that there are many components to the overall concept of mechanical response. In fact, FRAPCON uses FRACAS-I coupled with other non-specific thermal expansion models to develop an encompassing solution that describes the state of the fuel rod taking into account geometrical considerations. It involves a complex set of relationships describing geometry-dependent phenomena, region interfaces, and composition changes. At this point in the AM/MD model, such macroscopic phenomena are impossible to describe. For this reason, all FRAPCON AM/MD calculations will retain the geometry-dependent and burnup correction factors of FRAPCON, while the nature of the theoretical thermal expansion regimes is changed from the empirical FRAPCON model to the

first-principles AM/MD model. From a programming standpoint, this change may seem minor, but the substitution occurs in the most fundamental and physically significant section of code, and so therefore has the potential to have a profound effect on the overall performance of the code. To illustrate this point, Figure 2-6[3] gives a detailed flow chart of the overall FRAPCON process, highlighting the specific sections that are to be modified for the FRAPCON AM/MD model.

2.4.1 FRACAS-I Deformation Model

As mentioned previously, the FRACAS-I model is designed to analyze fuel and cladding mechanical deformation in order to better simulate the effects of burnup and temperature on the fuel pin. FRACAS can model two scenarios. The first of these is an "open gap" situation, when the fuel and cladding are not in contact. This "open gap" situation has cladding with internal and external pressures that must be calculated. The second scenario is when the fuel has expanded enough to be in contact with the cladding. In this "closed gap" situation, the fuel drives the cladding outwards. Overall, the calculations take into account the effects of fuel thermal expansion, fuel swelling, fuel densification, fuel relocation, cladding thermal expansion, cladding creep, cladding plasticity, and fission gas/external coolant pressures. Because the gap closure is a function of burnup, the FRACAS-I model determines gap thickness as a function of time, and determines the appropriate open-gap or closed-gap model. Fuel expansion leading to a closed gap depends on both thermal factors and radiation factors; thus, to properly calculate lifetime strain both the open gap and closed gap models were used for the analysis. At the current stage of analysis, no changes have been made to the gap conductance or fuel cladding regimes in the FRACAS-I model. The components of the FRACAS-I model which are not explicitly used to calculate the theoretical thermal expansion of the fuel pellet remain unchanged during this investigation, and as a result, they will not be covered here. This investigation is

concerned with the basic theoretical calculation of thermal expansion, which is discussed in the following section.

2.4.2 Fuel Thermal Expansion Subroutine

The subroutine within FRAPCON-3 that directly calculates the thermal expansion of the fuel is FTHCON.F, which is a subroutine called by FEXPAN.F in the FRAPCON source code.

$$\varepsilon = 10^{-5} \times T \; - \; (3.0 \times 10^{-3}) + \; (4.0 \times 10^{-2}) e^{(6.9 \times 10^{-20} / k_b \times T)} \quad \textbf{(1.11)}$$

This relationship describes the non-geometry dependent temperature-induced strain of UO_2, and is part of the FRACAS model. The thermal expansion study gives an indication of the sensitivity of the thermal expansion coefficient while maintaining the methodology for simulation of other macroscopic properties, and will continue to be studied as the MD model continues to be developed.

2.5 FRAPCON Code Description

This section presents an overview of the particular code structure of FRAPCON. Because FRAPCON is a product of over 50 years of development and modification, it contains over 200 modularized and independent subroutines. For this reason, it is favorable for the selection of particular subroutine modification, without causing catastrophic compilation errors, provided proper variable control is maintained.

FRAPCON consists of 3 major packages: the main FRPCON package, which calls all other packages and subroutines, the FRACAS-I package, which calls all components of the FRACAS-I mechanical model, and the MATPRO materials properties package. For the purposes of this investigation, both the FRACAS-I and MATPRO packages are to be modified, while the FRPCON package itself remains unchanged, to maintain fluidity. The hierarchy and

loops structure of the major code components is given in Figure 2-6, modified from the FRAPCON manual.[3]

The output of FRAPCON-3 is in the form of a substantial text file, giving thermal, mechanical, and pressure response data for each time/burnup step. The output file is organized into three sections: summary-page, axial-region printout, and power/time step printout. Boundary conditions for the beginning of each time step are explicitly printed into each power/time step section. Because so many calculations are performed at each radial node, axial node, region, and time step, the output files for each FRAPCON run are around 500 pages of text. In order to de-convolute this output, a plot package is included, which collects and plots 1-D and 2-D data, with selectable fields for the abscissa and ordinate. This plotting package is currently in the form of a MS excel spreadsheet, and contains both original data retrieval macros, and some modified for this project.

2.6 FRAPCON Input File

The input file used by FRAPCON is a text file explicitly defining a number of physical parameters, operation descriptors, evaluation model options, special flags, and isotopic distributions. Like many FORTRAN IV input files, a FRAPCON input file uses special characters and commands to evaluate the problem, read appropriate parameters, and create a robust output file.

For this investigation, it is important to note that the primary focus is to obtain a quantitative relationship between the unmodified FRAPCON program and a new, hybridized FRAPCON-AM/MD program for the same fuel rod. For this reason, the input file should have the same physical parameters in both the FRAPCON and FRAPCON-AM/MD cases. This is, in fact, the case, with only the output data fields being different for each case. The input file is included in Appendix A.

In order to establish a base case, an input file was chosen which models a typical fuel rod. The rod used for this investigation is Oconee Rod 15309, from the Oconee nuclear station near Greenville, South Carolina. Oconee is a three-unit nuclear power station owned by Duke Energy Corporation Company and operated by Duke Power Company which produced over 19 million megawatt hours of electricity per year as of 2003.[10] Unit 1 began operations in 1973, and the plant is licensed to operate until 2033. All three units are supplied by Babcock and Wilcox (now AREVA ANP).

For this investigation, 34 time steps are used, representing a burnup of 0 to 46.2 Megawatt days per kilogram Uranium (MWd/kgU), over a lifetime of 1550 days. Table 2-1 summarizes of the major parameters of the pellet in the FRAPCON input file:

Table 2-1 FRAPCON input parameters for Oconee rod model.

Number of time steps	34
Number of axial regions	12
Number of equi-volume radial rings	15
Pellet Density	95% theoretical density (td=10.96g/cm^3)
Enrichment	3% (atom %)
Pitch	1.4224 cm

In addition to the parameters listed on Table 2-1, it should be noted that no gadolinia was included in the fuel, and the fuel is presumed to be fresh, unirradiated UO_2. The MOX fuel case is also available in FRAPCON, but has not yet been investigated against an appropriate AM/MD model.

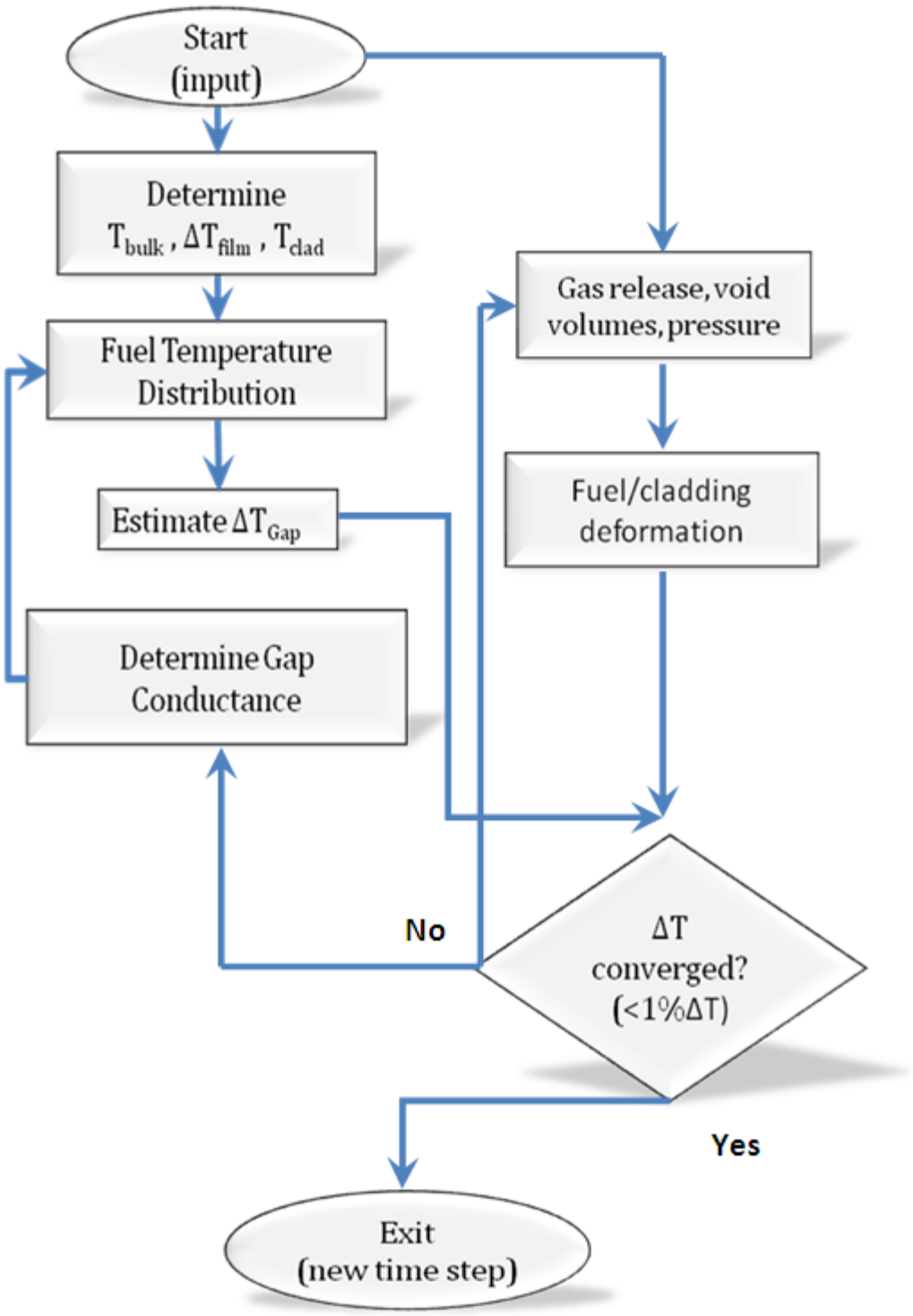

Figure 2-1. Simplified FRAPCON solution scheme for one time step

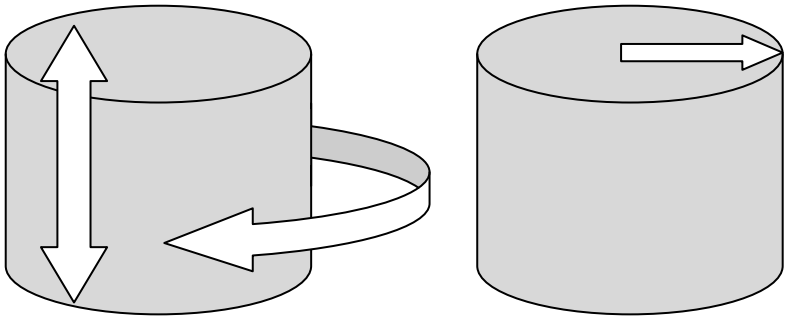

Figure 2-2. Temperature calculation for 1-D assumption

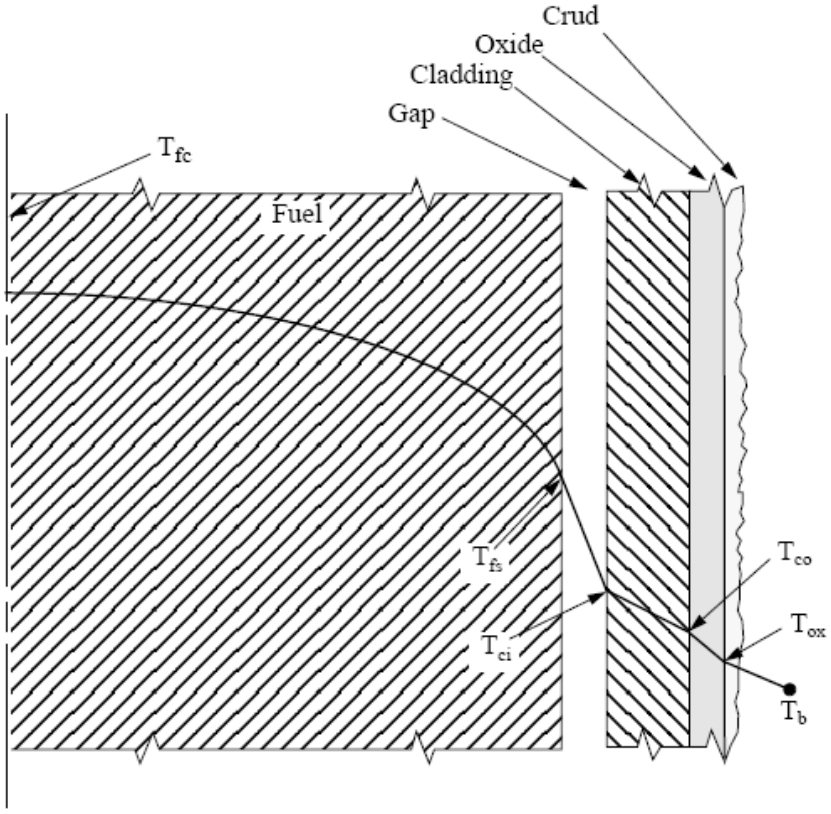

Figure 2-3.[3] Fuel rod temperature radial distribution

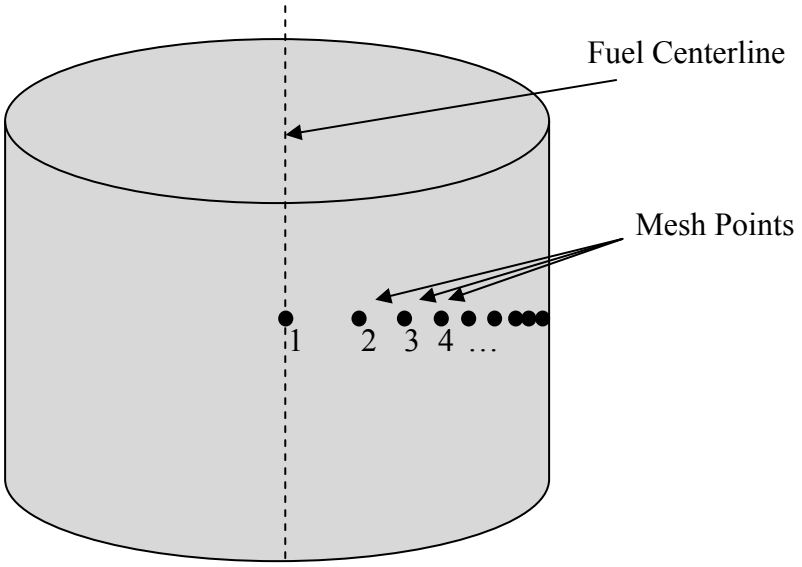

Figure 2-4. Mesh point layout

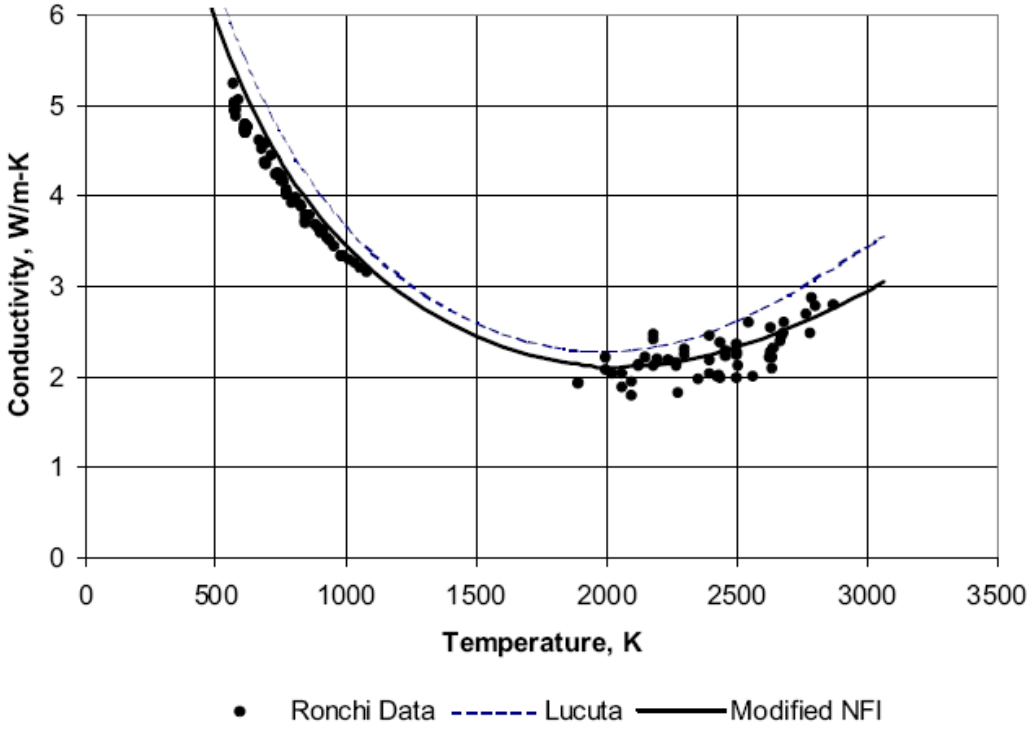

Figure 2-5.[7] FRAPCON conductivity functions with Ronchi data

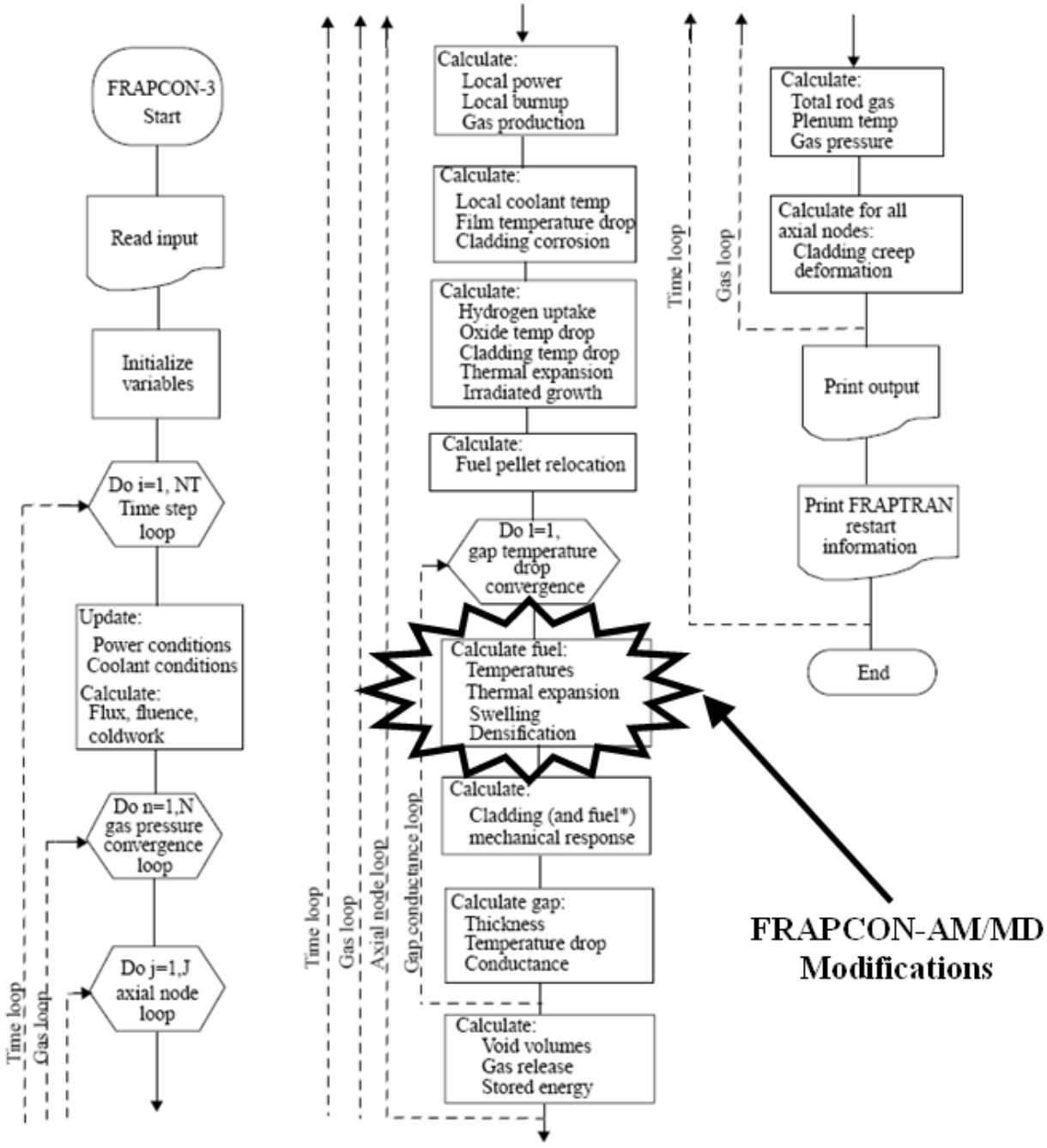

Figure 2-6.[3] FRAPCON solution schematic

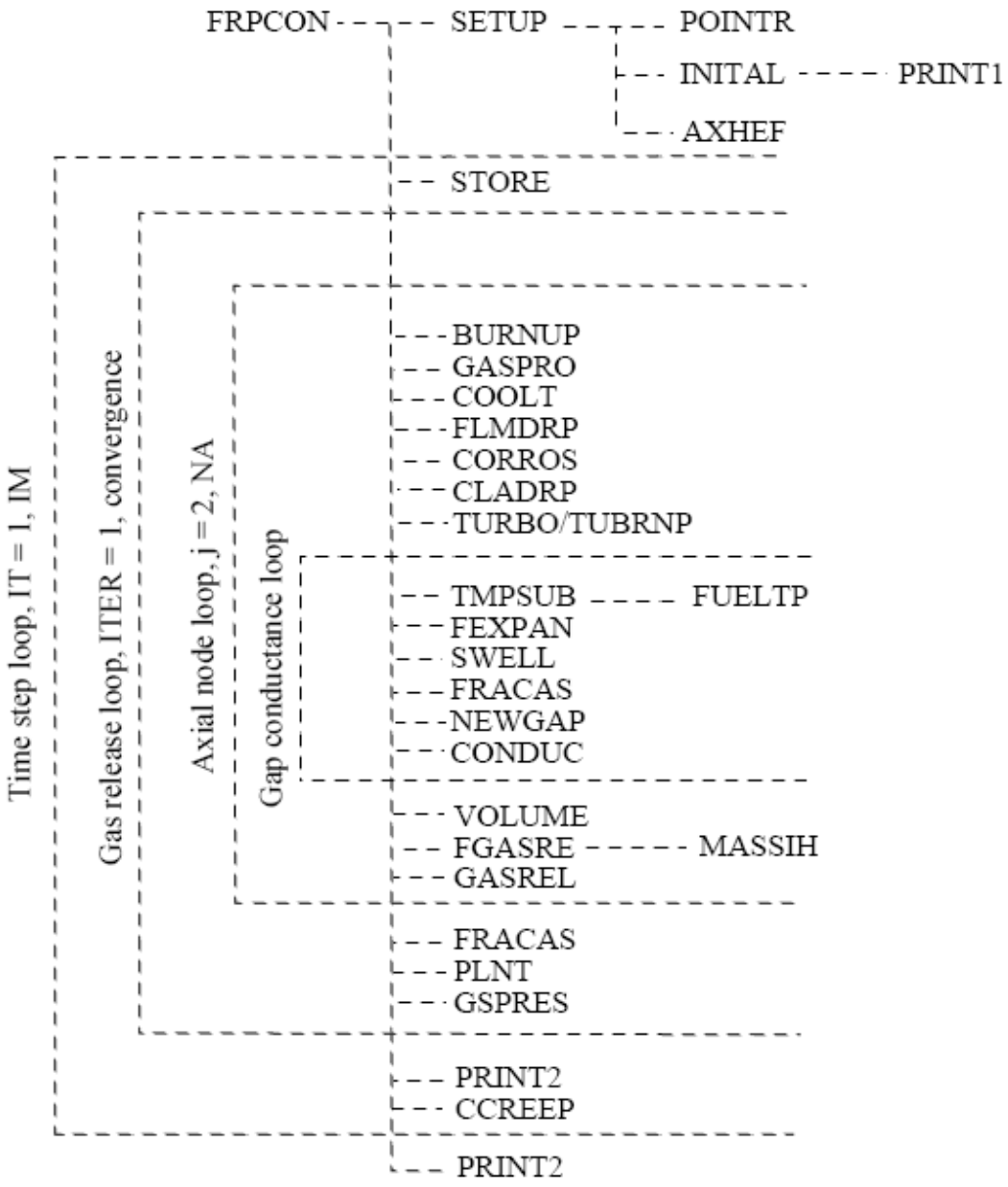

Figure 2-7. FRAPCON calling sequence. (boxed names are modified in AM/MD).

CHAPTER 3
MOLECULAR DYNAMICS MODELLING

The molecular dynamics model used in this investigation (AM/MD) will eventually describe components not necessarily included in a more generic MD case. Generally, MD models have been developed to describe statistical fluid mechanics, borrowing from mathematics, physics, and chemistry. As a way to produce a simulated experiment, of sorts, it has been called "statistical mechanics by numbers".[11]The AM/MD model presented in this investigation will eventually include an array of micro-structure components, both intrinsic and as a result of burnup. Phenomena such a fission gas production, fission product migration, chemistry/stoichiometry changes, and grain growth will be manifested as specific point-defects represented design parameters created in the AM/MD model. In this way, these fission-related phenomena, previously accounted for by empirical data correlations, can be represented by first-principles design in a never before seen manner.

3.1 Molecular Dynamics Simulation

Molecular-dynamics (MD) simulation is a well-developed computational methodology, widely used in the materials and physics communities for the simulation of the properties and behavior of materials with regard to stoichiometry and point defect changes.[12,13] In essence, MD simulation allows a finite number of particles to interact based on known laws of physics, and then uses the results to determine the overall properties of the system. Because of the complexity of molecular systems, it is often impossible to obtain materials properties by purely analytical methods. For this reason, MD simulation uses numerical methods to determine thermo-mechanical properties of a given system based on input parameters including time and position.

Traditionally, the procedure for MD simulation has been to examine a material at the lattice level, with the atoms treated as classical objects described by Newton's equations of motion. Each individual atom moves according to the net force exerted on it from all of the other atoms in the system; these forces are described in terms of an interaction potential, which is a relationship for the dependence of the energy and force on an atom due to the other atoms in the system. The mathematical form of the interatomic potential depends on the material simulated and is typically parameterized to experimental properties, such as the crystal structure, lattice parameter(s), elastic properties and other pertinent physical properties.

With the advent of more capable computational systems, MD simulations have become more efficient. Typically, these MD simulations model up to millions of atoms, allowing small, but finite amounts of material to be simulated. The effects of temperature and the dynamical evolution of the system can be captured in this approach in a natural way. More particularly, As described in detail in additional MD publications from the University of Florida Department of Materials Science and Engineering,[14,15,16] MD simulations have been used to characterize the thermal expansion and thermal conductivity of pure, defect-free UO_2. The results from such simulations are used in this investigation as modification to the FRAPCON source code.

3.2 The AM/MD Model Results

Based on the studies currently being carried out by the University of Florida Materials Science and Engineering Department, a number of MD simulations have been undertaken. For this investigation, the MD results of that study yielded specific best fit relationships for both the thermal conductivity and thermal expansion. These results have yielded a best fit equation for the instantaneous thermal conductivity given by Equation 2-1.

$$k_o = \frac{59848}{(2.38)} \times T^{(-1.291)} \qquad (2\text{-}1)$$

Equation 2-1 is used as the basis for calculating the simple thermal conductivity as a function of temperature. For the nominal temperature ranges associated with steady-state reactor operations (up to 1400 K), it is known that phonon-phonon interaction is the dominant form of heat transfer. The physical meaning of the single term in Equation 2-1 represents this phonon interaction, and it is expressed in Debye form: $k=(1/a+bT)$.[17] At higher temperatures, effects of polarons become increasingly significant, but for the purposes of this investigation, the polaron interactions are not included in the AM/MD model. As is evident from the equation, no realtionship between burnup and conductivity is given. This relationship is not yet explored by the AM/MD. Instead, the AM/MD will simply be substituted for equation 1-3 in the FRAPCON code. For the investigation of thermal expansion, the AM/MD model predicted

$$\varepsilon = 8.835\times10^{-6}T - 2.65\times10^{-3} \qquad (2\text{-}2)$$

According to the AM/MD simulation, the predicted thermal expansion does not change to any great extent for systems with point defects or polycrystalline microstructures. This is consistent with the FRACAS assumption of the independence of the thermal expansion on microstructure, and with experimental results on a wide range of materials.

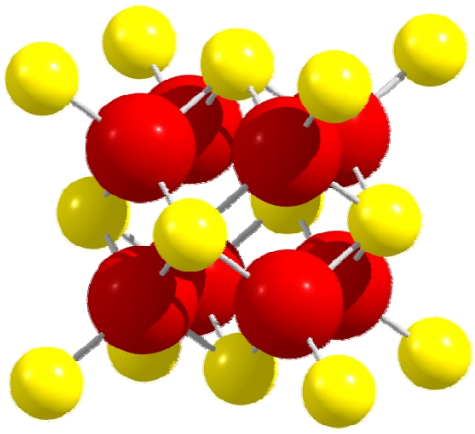

Figure 3-1. Typical UO_2 lattice for MD simulation

CHAPTER 4
SIMULATION METHODOLOGY

In essence, two virtually identical FRAPCON performance codes are created. The first, which provides a base case, is the original FRAPCON-3 source code, with all original conductivity and thermal expansion calculation algorithms in place. When this collection of source code it compiled, the compiler creates an executable FRAPCON file, which is initiated by the FRAPCON input file. The second case, the FRAPCON-AM/MD performance code is the project containing the modified thermal conductivity and expansion algorithms. In order to compare the reactor performance of the original FRAPCON and FRAPCON-AM/MD models, the same input file is used. This section explains the computational integration of the AM/MD model with the FRAPCON model

In order to effectively implement the results of the AM/MD simulation into the FRAPCON-3 code, it is important to establish continuity between the explicit definitions of the quantities to be modeled. In the case of thermal conductivity, it is important that because the AM/MD model predicts thermal conductivity only for fresh, un-irradiated fuel, that the FRAPCON simulation be run with a substitution for base conductivity, but that the embedded burnup and degradation effects not be changed. For thermal expansion, it is important that a normalized stress strain start point be established, so that FRAPCON has a known reference point for making the temperature-dependent stress/strain calculations required for each time step. The following sections explain how this implementation was carried out.

4.1 Thermal Conductivity FRAPCON/AMMD Implementation

The AM/MD equation established for thermal conductivity (equation 2-1) was compared to that of the Modified NFI thermal conductivity model given in the latest FRAPCON-3 release (equation 1-3), and it was found that in the pertinent temperature range of typical LWR

operations, there is relative consistency with both the magnitude and shape of the temperature/conductivity curve. While it is evident that the AM/MD model predicts a slightly higher conductivity up to 950K, and then a slightly lower conductivity at higher temperatures, these results would indicate that the model is sufficiently close for implementation into the FRAPCON-3 code. Figure 4-1 gives a plot of the conductivity predicted by FRAPCON/NFI method plotted against that obtained using the AM/MD simulation.

The source code file which controls the instantaneous base conductivity (prior to burnup phenomena modification) is a subroutine named FTHCON.F, and is called by the main FRPCON.F package which returns an instantaneous thermal conductivity value to the FRPCON.F routine. The input variables for this routine include current stage burnup, temperature of the radial ring, modified fuel density, and stoichiometry ratio (atoms-metal/atoms-oxide), producing an output of the instantaneous modified thermal conductivity. The value calculated for this conductivity is then output back to the overall thermal conductivity iterative loop, where burnup effects discussed in Section I.C.2. are manifested. The FTHCON.F source file can be found in its entirety in Appendix A. An excerpt of the modified FTHCON.F subroutine is given in figure 4-2.

4.2 Thermal Expansion FRAPCON-AM/MD Implementation

In order to properly implement the thermal expansion calculations associated with the AM/MD simulation, it is important to note the definitions given within both the FRAPCON code and AM/MD values. Within FRAPCON, a number of manifestations of thermal-induced stress and strain are given, including strains associated with components outside the fuel. For the cladding strain, no modifications were made to the code in order to maintain overall consistency with the two simulations. In the fuel pellet itself, there are a number of calculations carried out

by the FRACAS-I model, including axial strain, hoop strain, radial strain. In addition, the surface displacement and accumulated lifetime strain are also included.

In the case of the AM/MD model, there is no sense of dimensionality or UO_2 pellet shape; thus, the concept of thermal-induced strain is given in the context only of a change in the lattice parameter. While it is possible to assume equiaxial growth in each dimension, such as in the case of isotropic thermal expansion, it remains to be evaluated just how valid of an assumption this will ultimately lead to. At this point in the investigation, the lattice parameter expansion derived from the AMMD model will be substituted directly for the linear growth due to thermal expansion in FRAPCON.

The temperature-dependent lattice parameter expansion (equation 2-2), with a conversion into linear strain, as well as a zero-intercept adjustment to 300K derived from the AMMD simulation is given by equation 3-1 and plotted against that given in the FRACAS-I model (equation 1-11), and given in figure 4-3.

This plot shows that the two models exhibit similar behavior, but are not in quantitative agreement. This disagreement notwithstanding, it is useful to carry out a preliminary analysis of the effect of the thermal expansion model on the evolution of the system during burnup. The apparent inconsistency for predictions of the thermal expansion are a result of the rather poor materials fidelity of the interatomic potential used in the AM/MD simulations. While the AM/MD model is based on the work by Yamada, MD models more consistent with geometrical effects, as well as refinement of interatomic potentials with respect to stoichiometric changes and defect formation must be implemented in the future. For the proof of principle presented in this investigation, however, the AM/MD model will be used to produce a sensitivity analysis indicative of the effect of fuel thermal expansion on overall fuel performance. The

implementation of the thermal expansion model required slightly more changes be made within the FRAPCON code. Because the FRACAS-I model uses the thermal expansion to calculate macroscopic thermo-mechanical phenomena, it was important to modify only the thermal-induced swelling of the fuel, so that it could be integrated into FRAPCON as seamlessly as possible, and without interfering with the calculation of other thermo-mechanical phenomena already in place. To do this, the subroutine FEXPAN.F was modified to calculate thermal expansion from the AM/MD thermal expansion (equation 2-2). The FEXPAN.F subroutine is available in Appendix B.

While the thermal expansion properties of UO_2 are well known, this sensitivity analysis study is paramount in this investigation, because it allows for a radically independent model to describe a phenomenon, and gives the potential to do so for other materials which are as of yet, not as well known.

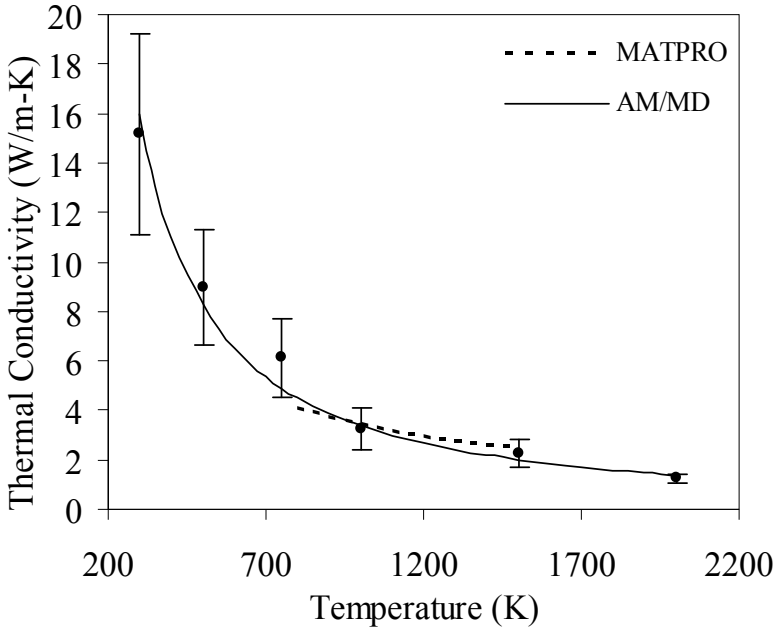

Figure 4-1. Thermal conductivity predicted by FRAPCON and AM/MD calculations.

```
*deck fthcon

            subroutine fthcon (ftemp,fraden,fotmtl,con,burnup
           + ,gadoln,imox)
      c   fthcon calculates the fuel thermal conductivity and its
      c   derivative with respect to temperature as a function of
      c   temperature, density, composition and burnup.
      c   UO2 Fuel (IMOX = 0)
      c   The equation used in this subroutine is that proposed by
      c   staff at NFI, Japan, at the May 1997 ANS Topical Meeting on
      c   Light Water Reactor Fuel performance in Portland, OR: (Ohira,
      c   K., and N.Itagaki, 1997.  "Thermal Conductivity Measurements
      c   of High Burnup UO2 Pellet and a Benchmark Calculation of Fuel
      c   Center Temperature", proceedings pp. 541-549. Applies to UO2.
      c   burnup = current local burnup (MWd/MTU)
      c   con    = output fuel thermal conductivity (W/(m*K))
      c   ftemp  = current fuel ring temperature (K)
      c   fraden = input fuel density (ratio of actual density to
      c            theoretical density)
      c   fotmtl = input oxygen to metal ratio of fuel (atoms oxygen/
      c            atoms metal)
      c   gadoln = input weight fraction of gadolinia in the fuel
      c
      c   the following inputs are by common block
      c   comp   = input puo2 content of fuel (percent puo2
      c            in total fuel weight)
      c   bu     = input burnup (mw-s/kg-u)
      c Verify subroutine entered
      c write (*,*) 'Entered fthcon.f'
      c
      c   find constants:
      c      frpu = comp/100.
             t = ftemp
      c
      c  Burnup in GWd/MTU
      c
             bug = burnup/1000.0
      c
             if(imox.eq.0) then
      c
               h = 1/(1.0+396.0*exp(-6380.0/t))
               rphonon= 1.0/(0.0452+0.000246*t + 1.0*0.00187*bug+1.1599*gadoln
           &  + (1.0-0.9*exp(-0.04*bug))*0.038*bug**0.28*h)
               elect = (3.50e9/t**2)*exp(-16361/t)
      ******************************************************
      C CORRELATION GIVEN BY AM/MD (3/2/2007)
      C
        base=59848*ftemp**(-1.291)/2.38
      ******************************************************
                fm  = fraden/(1.0 + 0.5*(1.0-fraden))
                con = base*fm*1.079
      ******************************************************
      c CORRELATION GIVEN BY FINK ----> NOTE: FOR 95% DENSE
      c
      c        con = 100/(6.548+25.533*(ftemp/1000))
      c     &  + 6400/((ftemp/1000)**(5/2))*exp(-16.35/(ftemp/1000))
      ******************************************************
      c
      c   find uncertainty
             if(imox.eq.0) then
               if(t.lt.ftmelt) then
                 ucon = 0.2*(1.0+abs(2.0-fotmtl)*10.)
               else
                 ucon = con/2.0
               endif
             else
               if(t.le.1800.0) then
                 ucon = 0.07*con
               else
                 frac=(t-1800.0)/(3100.0-1800.0)*(0.20-0.07)+0.07
                 ucon=frac*con
               endif
             endif
             if (emflag(locidx).eq.on) call emfton (ftemp,fraden,ftmelt,con)
             return
             end
```

Figure 4-2. Modified FTHCON.F code excerpt

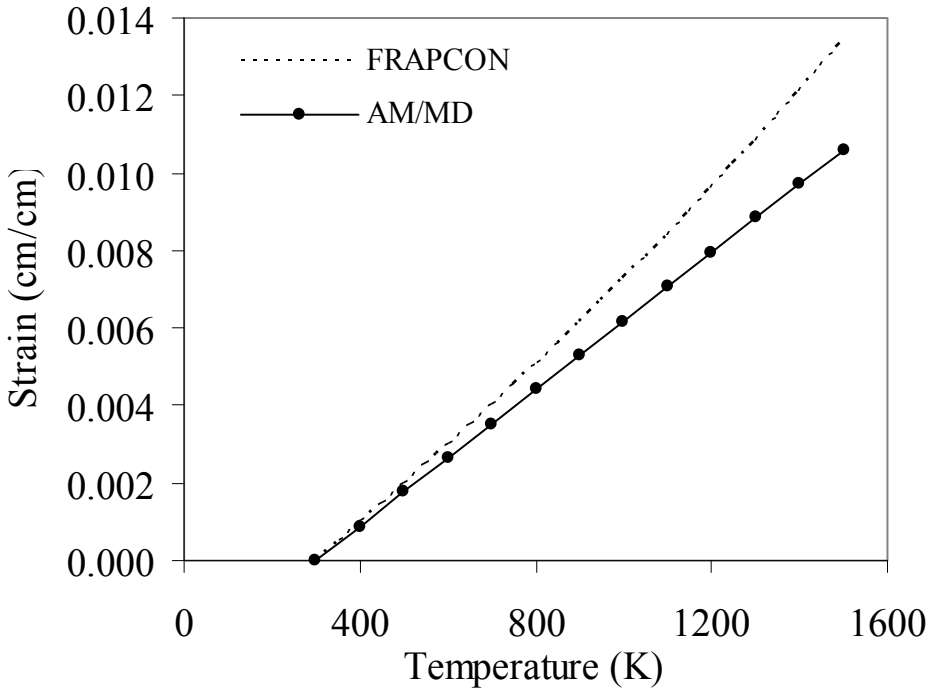

Figure 4-3 Temperature-dependent strain for FRACAS-I and AM/MD. (relative to 300K).

CHAPTER 5
RESULTS AND OUTLOOK

5.1 FRAPCON-AM/MD Conductivity Results

The first and most direct method by which to analyze the AM/MD model implanted into the FRAPCON code is to analyze the Beginning of Life (BOL) temperature profile at full power. This situation has a real world analogy to the situation in which a reactor comes online for the very first time at full power, with burnup essentially zero.

In order to do this, data was mined from the output file given by the FRAPCON executable, and plotted using a data extraction macro in Microsoft Excel. Because FRAPCON uses a 1-D, multi node approach, each axial and radial node distinct temperature distributions. The For the sake of simplicity, the limiting case was taken. For both the FRAPCON and FRAPCON-AM/MD cases, the 'hottest' node was axial node 4 of 12. The corresponding output obtained for the full power/zero-burnup cases, with corresponding heat generation rates, is given in Appendix D. Figure 5-1 compares the radial temperature profiles for the FRAPCON and FRAPCON-AM/MD cases. It is clear from this figure that while the centerline temperature is slightly lower for the AM/MD case (i.e, the conductivity is slightly overestimated), the temperature distribution is very consistent in both cases. Such a result would be expected based on the fact that the FRAPCON model contains similar thermal conductivity function obtained by the AM/MD model.

Perhaps the most encouraging part of this finding is that the interatomic potentials used in the AM/MD have been successful in calculating the thermal conductivity of fresh UO_2 fuel in a radically independent way from that used in FRAPCON, yet yield nearly identical fuel performance. Because of the nearly identical chemical properties of uranium and plutonium, UO_2 and PuO_2 have the same fluorite crystal structures, similar melting points, etc. For this

reason, the possibility exists to manipulate the AM/MD model in such a way as to either systematically or randomly substitute Pu cations for U cations, adding another set of interatomic potentials, and thus creating a MOX fuel simulation with very little additional effort. In the future, it is expected that other, more exotic fuels, such as SiC and other inert matrix fuels will be modeled using MD methods.

5.2 FRAPCON-AM/MD Thermal Expansion Results

After restoring the original FRAPCON conductivity and modifying the FEXPAN.F subroutine, the same procedure as that done with the thermal conductivity was carried out. Namely, that two executable files were created; one for the FRAPCON case, and one for the FRAPCON-AM/MD case. For this comparison, it was determined that a good indication of the sensitivity of the system to thermal-induced expansion could be evaluated in the context of both instantaneous and burnup-dependent conditions. More particularly, fuel relocation and irradiation-induced swelling become increasingly significant compared to thermal-induced swelling as the life cycle of the fuel proceeds. This is evident in the apparent convergence of surface displacement calculations near 900 Full power days (~27 MWd/kgU).

The results from 5-2 show the densification of fuel for the first few burnup steps, as well as the prescribed burnup effects evident from empirical correlations given in FRAPCON. While two models exhibit similar behavior, they are not in quantitative agreement. This disagreement notwithstanding, this preliminary analysis of the effect of the thermal expansion model on the evolution of the system during burnup is useful in determining a qualitative feel for the degree to which burnup phenomena vs. thermal expansion affect the strain conditions of the fuel pellet. Rigorous studies of the nature of these burnup phenomena have been done, and are continuing to be developed. It is a major ultimate goal of this AM/MD project to be able to simulate these burnup effects from a first-principles standpoint using MD models. Such a model

would incorporate not only stoichiometry conditions and interatomic potentials, but transmutation (radiative capture), grain boundary restructuring, fission gas release, high energy radiation particle damage, and their relationships to defect formation. Macroscopic phenomena, such as geometrical concerns and fuel flaking/cracking present unique challenges that may not be suitable for MD modeling. Such questions remain to be determined by further research on this AM/MD project.

5.3 Proposed AM/MD Modifications

It is clear that in order to rectify the issues with thermal expansion, a more in-depth AM/MD model will be required. Fortunately, the integration of such a model has been proven to be a straightforward process, and it can be taken into consideration piece by piece. It has been shown in a recent study (Govers, 2007) that current interatomic potentials lack the fidelity required to compete with detailed experiments[18]. A primary step in the development of this model will be the continued development of higher fidelity potentials, which can be integrated into the code. A second major step in development of this project is the rigorous evaluation of proper infiltration of MD models into FRAPCON. This will come with an increased emphasis on developing MD models in a functional form capable of coupling prudently with FRAPCON.

The third and ultimate proposals for the AM/MD model is the incorporation of degradation and burnup phenomena, as well as radiation and fission event effects in the context of MD. A model must be created such that in intact lattice suffers a displacing fission event, creating high energy fission products as well as secondary radiation particles, lattice vacancies, interstitials, stoichiometric changes, production of fission gasses/porosity and fuel swelling/densification. By assigning a weight determined through sensitivity analysis to each of these phenomena, either a numerical or a Monte Carlo model be created to simulate the radiative capture and/or fission of a single atom. Figure 5-3 shows a purely conceptual example of how a fission event may change a

lattice. With such a model created, the avenue will be set for creating MD-based inert matrix fuel performance calculations.

5.4 Conclusions and Recommendations

In summary, this work is successful in providing provides a proof-of-principle that a fuel performance code can be adapted to accept input from atomistic model simulations. A very significant amount of further research is, however, required before atomistic models can reliably supplement, let alone overtake accuracy obtained by detailed experiments. As mentioned in the previous section, the direct comparisons with base FRAPCON results show current AM/MD models cannot yet provide inputs of sufficient materials fidelity to be quantitatively predictive. Such materials fidelity is only achievable by continued research in improvement of interatomic potentials.

It is also clear that AM/MD model agrees far better with the FRAPCON's overall prediction of BOL characteristics than it does with the simple thermal conductivity model for UO_2 itself. For the thermal expansion the rather significant deviation of the AM/MD model from the FRAPCON model is not manifested in the surface displacement for the first 100 days, after which, issues related to code implementation may become more profound. These issues will be addressed in continued development of this project.

The two properties addressed in this investigation are likely the most simple to integrate into a fuel performance code, but are in addition the most important. The sizable challenge faced in developing an atomistically informed fuel-performance code is that of incorporating the complexities associated with the changing chemistry associated with such effects as fuel swelling, fuel densification, fuel relocation, cladding thermal expansion, cladding creep, cladding plasticity, and fission gas release.

In more general and far-reaching terms, the development of multi-scale models such as the integrated FRAPCON-AM/MD is intended to ultimately help optimize the nuclear fuel materials selection process through atomic level molecular dynamics (MD) involving first-principles materials simulations. It is a goal of this investigation that a robust method by which nuclear fuel will be selected can be created by understanding performance sensitivities exposed by MD simulation. Incorporation of such a process will minimize the need for expensive and time-consuming in-reactor experimental testing.

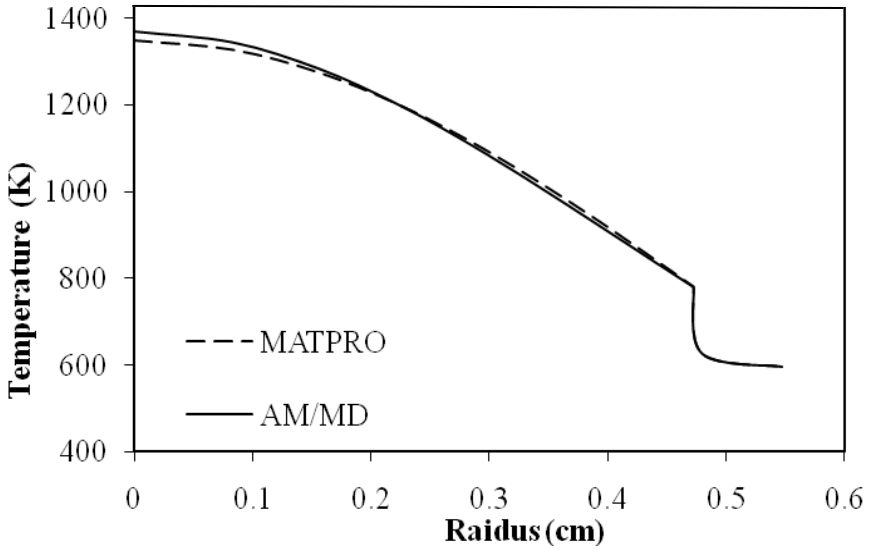

Figure 5-1. Pellet temperature profile for MATPRO and AM/MD cases at BOL

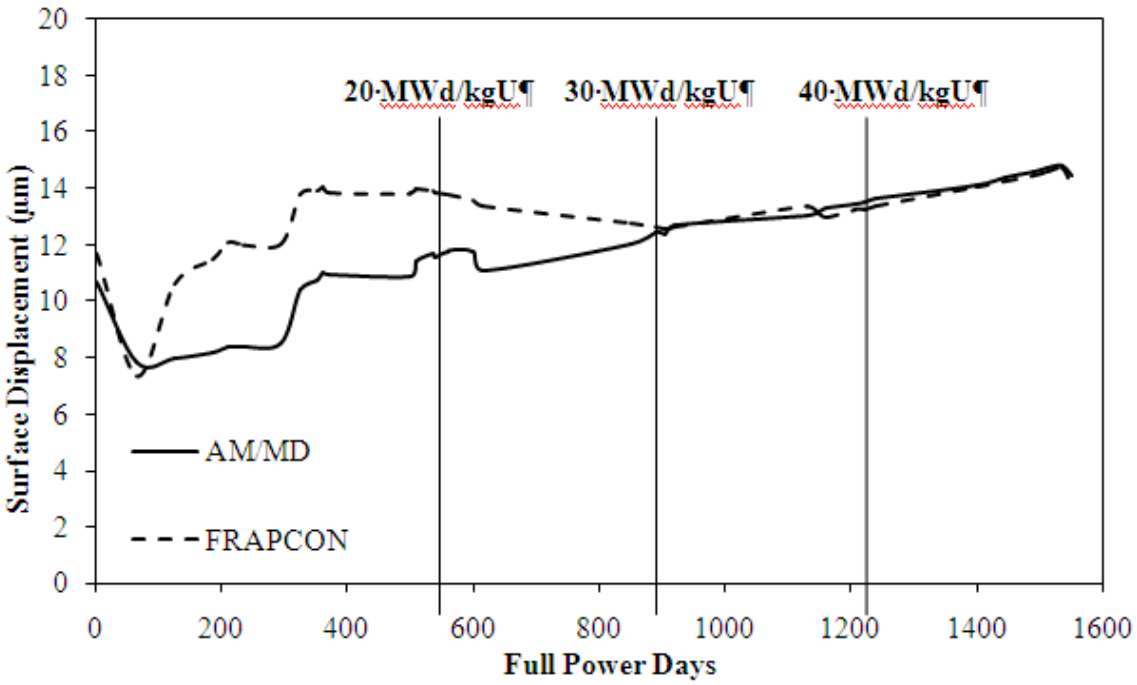

Figure 5-2. . Lifetime surface displacement of fuel pellet

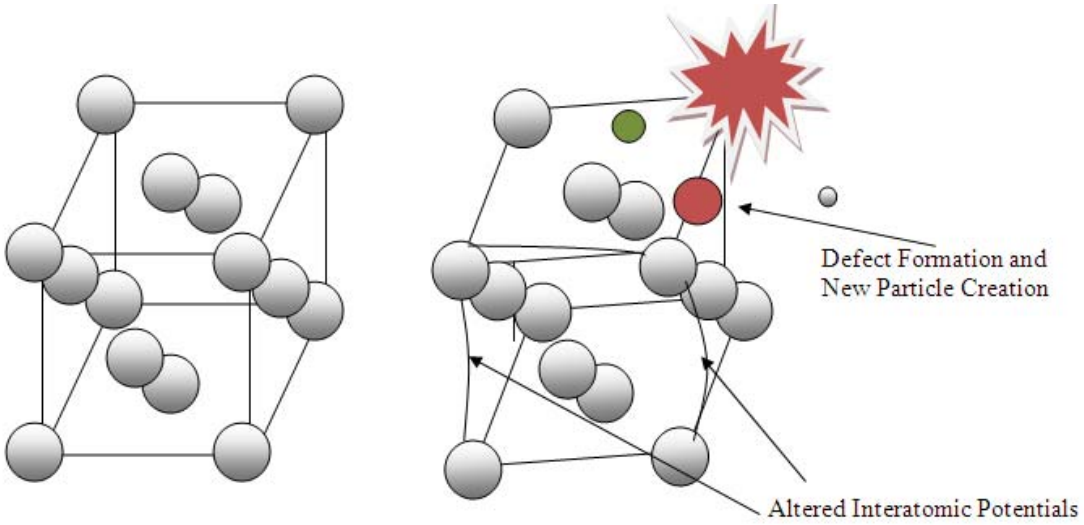

Figure 5-3. Conceptual model of fission event and lattice effects

APPENDIX A
FTHCON.F SOURCE FILE

```
*deck fthcon

      subroutine fthcon (ftemp,fraden,fotmtl,con,burnup
     + ,gadoln,imox)
c
c   fthcon calculates the fuel thermal conductivity and its
c   derivative with respect to temperature as a function of
c   temperature, density, composition and burnup.
c
c   UO2 Fuel (IMOX = 0)
c
c   The equation used in this subroutine is that proposed by
c   staff at NFI, Japan, at the May 1997 ANS Topical Meeting on
c   Light Water Reactor Fuel performance in Portland, OR: (Ohira,
c   K., and N.Itagaki, 1997.  "Thermal Conductivity Measurements
c   of High Burnup UO2 Pellet and a Benchmark Calculation of Fuel
c   Center Temperature", proceedings pp. 541-549. Applies to UO2.
c
c   MOX:
c
c   Option number 1 (IMOX = 1)
c
c   The 100% dense solid MOX fuel thermal conductivity formulation is based
c   on a combination of the Duriez stoichiometry-dependent correlation,
c   derived from diffusivity measurements on unirradiated fuel pellets
c   (C.Duriez, et al, J.Nuclear Materials 277, 143-158 2000) and the burnup
c   degradation conatined in a modified version of the NFI fuel thermal
c   conductivity model
c
c   Option number 2 (IMOX = 2)
c
c   The MOX fuel thermal conductivity formulation is based
c   on the OECD Halden Reactor Project report "Thermal Performance of
c   of High Burnup Fuel  In-pile Temperature Data and Analysis"
c   W.Wiesnack, T. Tverberg, Proceedings of the 2000 International
c   Topical Meeting on LWR Fuel Performance
c
c
c   *********MODIFICATION: Daniel Vega (2006/2007)**********************
c
c   Option number 3 (IMOX = 3)
c
c       For now, the MOX fuel thermal conductivity formulation will be given
c       an arbitrary and unrealistic value. This will be used to verify that
c       FRAPCON will still run properly when IMOX is nither 1 nor 2. i.e., that
c       IMOX is of the correct data type to accept 1, 2, or 3.
c
c   ****************************************************************
c
c   burnup = current local burnup (MWd/MTU)
c   con    = output fuel thermal conductivity (W/(m*K))
c   ftemp  = current fuel ring temperature (K)
c   fraden = input fuel density (ratio of actual density to
c            theoretical density)
c   fotmtl = input oxygen to metal ratio of fuel (atoms oxygen/
c            atoms metal)
c   gadoln = input weight fraction of gadolinia in the fuel
c
c   the following inputs are by common block
c   comp   = input puo2 content of fuel (percent puo2
c            in total fuel weight)
c   bu     = input burnup (mw-s/kg-u)
c   emflag(12) = input switch for evaluation model. if this
c   variable is equal to 1.0, the matpro model for
c   fuel thermal conductivity is replaced by the
c   subcode emfton
c

       common  / phypro / ftmelt,fhefus,ctmelt,chefus,ctranb,
     +                    ctrane,ctranz,fdelta,bu,comp,deloxy
c
      include 'lacmdl.h'
      data      on       / 1 /,
     +          off      / 2 /,
     +          locidx   /  12     /
c
```

```
c       Verify subroutine entered
c       write (*,*) 'Entered fthcon.f'
c
c   find constants
c
       frpu = comp/100.
       t = ftemp
c
c  Burnup in GWd/MTU
c
       bug = burnup/1000.0
c
       if(imox.eq.0) then
c
c    NFI formula (Ohira & Itagaki, ANS LWR Fuel perf. Topical mtg. 1997)
c     MODIFIED in January 2002 to raise low-burnup thermal conductivity
c     at low temperature and lower thermal conductivity at very high temp.
c
         h = 1/(1.0+396.0*exp(-6380.0/t))
         rphonon= 1.0/(0.0452+0.000246*t + 1.0*0.00187*bug+1.1599*gadoln
     &   + (1.0-0.9*exp(-0.04*bug))*0.038*bug**0.28*h)
         elect = (3.50e9/t**2)*exp(-16361/t)
*****************************************************
C       STANDARD FRAPCON HALDEN CORRELATION
c        base = rphonon + elect
c
*****************************************************
*****************************************************
C       CORRELATION GIVEN BY TAKU WATANABE (3/2/2007)
C
        base=59848*ftemp**(-1.291)/2.38
C
C
*****************************************************
                fm  = fraden/(1.0 + 0.5*(1.0-fraden))
                con = base*fm*1.079
*****************************************************
c       CORRELATION GIVEN BY FINK ----> NOTE: FOR 95% DENSE
c
c               con = 100/(6.548+25.533*(ftemp/1000))
c     & + 6400/((ftemp/1000)**(5/2))*exp(-16.35/(ftemp/1000))
*****************************************************

c   fm is the Lucuta porosity correction factor(applied to 100% TD fuel)
c


c
c  NFI base equation is for 95% TD fuel, so multiply by 1.079 to
c   raise to 100% TD fuel conductivity, then multiply by fm
c


c
       else if(imox.eq.1) then
c       write (*,*) 'IMOX = 1'
c
c  Using the Duriez/NFI Mod correlation combination
c
c      base term for MOX
c      where X = deviation from stoichiometry (2-O/M)
       fm = 1.0789*fraden/(1.0+0.5*(1.0-fraden))
c fm is multiplied by 1.0789 to account for 95% TD
c Porosity correction is Lucuta correction, not Maxwell-Euken
c as proposed by Duriez et al.
       x = 2.0-fotmtl
       ax=2.85*x+0.035
       cx=(2.86-7.15*x)*1.0e-4
c
       h = 1/(1.0+396.0*exp(-6380.0/t))
       rphonon = 1.0/(ax + cx*t + 0.00187*bug+1.1599*gadoln
      &+ (1.0-0.9*exp(-0.04*bug))*0.038*bug**0.28*h)
       elect = (1.50e9/t**2)*exp(-13520/t)
       base = rphonon + elect
       con = base*fm
c
       else if(imox.eq.2) then
c
c       Using the Halden correlation
c
       tc=t-273.15
       tco=min(1650.0,tc)
       buguo2=bug*0.8815
```

```
      fm = 1.0789*fraden/(1.0+0.5*(1.0-fraden))


      base=0.92/(0.1148+0.004*buguo2+1.1599*gadoln+
     &    2.475e-4*(1.0-0.00333*buguo2)*tco)+
     &    0.0132*exp(0.00188*tc)

      con=base*fm
c
c      else if (imox.eq.3) call newmodule(ftemp,fraden,fotmtl,con,burnup,gadoln)
      else if(imox.eq.3) then
!      call newmod(ftemp,fraden,fotmtl,con,burnup,gadoln)
c
c    NFI formula (Ohira & Itagaki, ANS LWR Fuel perf. Topical mtg. 1997)
c     MODIFIED in January 2002 to raise low-burnup thermal conductivity
c     at low temperature and lower thermal conductivity at very high temp.
c
        h = 1/(1.0+396.0*exp(-6380.0/t))
        rphonon= 1.0/(0.0452+0.000246*t + 1.0*0.00187*bug+1.1599*gadoln
     &  + (1.0-0.9*exp(-0.04*bug))*0.038*bug**0.28*h)
        elect = (3.50e9/t**2)*exp(-16361/t)
        base = rphonon + elect
c
c   fm is the Lucuta porosity correction factor(applied to 100% TD fuel)
c
        fm  = fraden/(1.0 + 0.5*(1.0-fraden))
c
c  NFI base equation is for 95% TD fuel, so multiply by 1.079 to
c   raise to 100% TD fuel conductivity, then multiply by fm
c
        con = base*fm*1.079
c      write(*,*) 'cond = ', con
c      arbitrary value insertion for con (W/m-K)
c      con=1
c
c   If IMOX.ne.0,1,2,3 then stop the calculations
c
        else
        stop 'fthcon - IMOX not within bounds'
      end if
c      write(*,*) 'cond = ', con
c
c   find uncertainty
      if(imox.eq.0) then
        if(t.lt.ftmelt) then
          ucon = 0.2*(1.0+abs(2.0-fotmtl)*10.)
        else
          ucon = con/2.0
        endif
      else
        if(t.le.1800.0) then
          ucon = 0.07*con
        else
          frac=(t-1800.0)/(3100.0-1800.0)*(0.20-0.07)+0.07
          ucon=frac*con
        endif
      endif
      if (emflag(locidx).eq.on) call emfton (ftemp,fraden,ftmelt,con)
      return
                                              end
```

APPENDIX B
FEXPAN.F SOURCE FILE

```
*deck fexpan
c
      subroutine fexpan (ftmelt,sumexp,nr,nrm1,tfr,tfring,uo2exp
     +                  ,afal,crad,j,na,dph)
c   implicit real * 8 (a-h,o-z)
c   ******************************************************************
c   fexpan is called from frpcon and computes the therm exp of fuel
c   this subroutine was coded by g a berna in march 1978.
c   ******************************************************************
c   input arguments
c   ******************************************************************
c   afal   - additional thermal expansion factor
c   ftmelt - fuel melt temperature (K)
c   j      - axial node index
c   nr     - maximum number of radial nodes
c   na     - number of axial nodes plus one
c   nrm1   - nr - 1
c   crad   - cold state radii of fuel radial nodes (in)
c   tfring - fuel ring temperatures (F)
c   tfr    - radial node temperatures (F)
c   ******************************************************************
c   output arguments
c   ******************************************************************
c   dph    - thermally expanded pellet diameter (in)
c   sumexp - total fuel surface displacement due to thermal expan.(in)
c   uo2exp  - thermal expansion (in/in)
c   ******************************************************************
      real radn, alphaT
c      CURRENTLY THERE ARE 17 RADIAL NODES --> nr = 17
       dimension     tfr(50)  ,tfring(50)  ,crad(50) ,uo2exp(50,21)
c      write(*,*) 'nr: ', nr
      sumexp = 0.e0
          do 100 l=1,nrm1
          tfring(l) = 0.5*(tfr(l) + tfr(l+1))
          tfringk = (tfring(l) + 459.67)/1.8 !convert F to K
          facmot = 0.0
          if (tfringk.gt.ftmelt) facmot = 1.0

c      ******************ORIGINAL******************
c      write(*,*) tfringk
      uo2exp(l,j-1) = fthexp(tfringk,facmot) * afal

c      ******************************************
c      *************NERI MOD*************
c      write(*,*) afal
c      uo2exp(l,j-1) = 8.835e-6*tfringk-2.650497690e-3
c      *************NERI MOD*************

c      *************FINK'S MOD*************
c      if (tfringk.le.923) then
c      uo2exp(l,j-1) = (9.828e-6)-(6.93e-10)*tfringk+(1.33e-12)
c    &*tfringk**2-(1.757e-17)*tfringk**3
c      else if (tfringk.gt.923) then
c      uo2exp(l,j-1) = (1.1833e-5)-(5.013e-9)*tfringk+(3.756e-12)
c     &*tfringk**3-(6.125e-17)*tfringk**3
c      end if
c      uo2exp(l,j-1) = uo2exp(l,j-1)*tfringk
c      *************FINK'S MOD*************

c      write(*,*) 'temp: ', tfringk,'th.exp: ',uo2exp(l,j-1)

c         write(*,*) 'tfring=',tfring(l),'FRAP=',uo2exp(l,j-1)
c              alphaT=8.835*tfring(l)*0.000001
c              write(*,*) 'MD=',alphaT, 'ratio: ', uo2exp(l,j-1)/alphaT

          sumexp=sumexp+(crad(l)-crad(l+1))*(1.e0+uo2exp(l,j-1))
100       continue

c      write(*,*) 'uo2exp', uo2exp
       radn=dph/2
      sumexp = sumexp + crad(nr) * (1.e0 + uo2exp(nrm1,j-1))
c      write(*,*) 'temp(1): ', tfr(1),'rado: ',crad(1),
c     &'radn', radn
      dph = sumexp * 2.e0
      return
      end
```

APPENDIX C
FRAPCON AND FRAPCON-AM/MD INPUT FILE

```
*************************************************************************
*        frapcon3, steady-state fuel rod analysis code, version 1       *
*---------------------------------------------------------------------  *
*                                                                       *
*         CASE DESCRIPTION: Test Case Oconee Rod 15309                  *
*                                                                       *
*UNIT     FILE DESCRIPTION                                             *
*----     ----------------------------------------------Output:        *
*         Output :                                                      *
*    6        STANDARD PRINTER OUTPUT                                   *
*                                                                       *
*         Scratch:                                                      *
*    5        SCRATCH INPUT FILE FROM ECH01                             *
*                                                                       *
*  Input:   FRAPCON2 INPUT FILE (UNIT 55)                               *
*                                                                       *
*************************************************************************
* GOESINS:
FILE05='nullfile', STATUS='scratch', FORM='FORMATTED',
        CARRIAGE CONTROL='LIST'
*
* GOESOUTS:
FILE06='test.out',    STATUS='UNKNOWN', CARRIAGE CONTROL='LIST' *test
FILE66='test.plot',    STATUS='UNKNOWN', CARRIAGE CONTROL='LIST'
/*************************************************************************
        Oconee rod 15309
 $frpcn
 im=34, na=12,
 ngasr = 15,
 $end
 $frpcon
 cpl = 10.5, crdt = 0.2, crdtr = 0.0, thkcld = 0.0265,
 dco = 0.430, pitch = 0.56,
 den = 95., thkgap=0.0050, dishsd = 0.050,dspg = 0.37,
 dspgw = 0.055, enrch = 3., fa= 1.0, fgpav = 480,
 hplt = 0.70, hdish = 0.014, icm = 4,
 icor = 0, idxgas = 1, imox = 0, iplant =-2, iq = 0, jdlpr = 0,
 totl = 11.75, jn = 13,13,13,13,13, jst = 7*1,10*2,2*3,5*4,10*5
 rc = 0.0, roughc = 1.97e-5, nplot = 1,
 roughf = 2.36e-5, vs = 20.0,
 nunits = 1, rsntr = 150.,
 qf(1)=0.2,1.0,1.2,1.25,1.25,1.22,1.2,1.16,1.14,1.06,.78,.3,.15,
 qf(14)=0.2,1.08,1.18,1.12,1.04,0.97,0.97,1.00,1.03,1.05,1.10,0.97,0.2,
 qf(27)=0.2,0.82,1.02,1.11,1.13,1.08,1.04,1.05,1.14,1.19,1.13,0.9,0.2,
 qf(40)=0.2,0.95,1.05,1.03,1.03,1.08,1.12,1.12,1.1,1.05,1.0,0.81,0.4,
 qf(53)=0.45,0.94,1.02,1.05,1.07,1.10,1.12,1.11,1.10,1.06,1.02,0.95,0.5
 x(1)=0,1,2,3,4,5,6,7,8,9,10,11,11.75
 x(14)=0,1,2,3,4,5,6,7,8,9,10,11,11.75
 x(27)=0,1,2,3,4,5,6,7,8,9,10,11,11.75
 x(40)=0,1,2,3,4,5,6,7,8,9,10,11,11.75
 x(53)=0,1,2,3,4,5,6,7,8,9,10,11,11.75
 flux = 13*0.25e17, p2(1) = 2200.0, tw(1) = 555.0, go(1) = 2.6e6,
 ProblemTime= 0.1,65,125,185,210,235,295,
 325,350,360,370,500,510,535,540,560,600,
 615,850,
 890,905, 920,1130,1150,
 1160,1205,1220,1240,1400,1445,1490,1510,1535,1550,
 qmpy = 5.8,5.8,7.9,7.5,7.3,6.8,6.6,
 7.9,7.6,7.4,6.9,6.6,6.1,6.7,6.0,6.6,6.1,
 4.1, 5.4,
 5.1,4.7,5.4,5.0,4.5,
 4.3,4.4,4.3,4.4,4.5,4.55,4.6,4.65,4.7,3.6,
 slim = .05,
 $end
```

APPENDIX D
BOL RADIAL TEMPERATURE DISTRIBUTIONS

D.1 FRAPCON BOL Radial Temperature Profile (node 4/12):

```
 xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
 x                    **** FRAPCON-3.3 (Aug. 12 05) ****                    x
 x                         Released August   2005                         x
 x          Oconee rod 15309                                               x
 x                  run date:  07-Oct-30          page    7                 x
 xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

                        axial region number  4          power-time step   1

   avg.  linear heat rating, kW/m(kW/ft)    19.03(  5.80)
   local linear heat rating, kW/m(kW/ft)    23.94(  7.30)          rod surface heat flux, W/m**2(btu/hr-ft**2)
6.97E+05(2.21E+05)
   peak  linear heat rating, kW/m(kW/ft)    23.93(  7.29)

   step starts at time, days(sec)     0.00( 0.00E+00)              starting burnup,  MWd/kgU(MWd/mtU)    0.00(     0.)
   time increment,      days(sec)     0.10( 8.64E+03)              burnup increment, MWd/kgU(MWd/mtU)    0.00(     4.)
   end step,            days(sec)     0.10( 8.64E+03)              end step burnup,  MWd/kgU(MWd/mtU)    0.00(     4.)

                                  Radial temperature and power distribution

                                          Radii , cm(in)                Temperature, K(F)   Power profile

                      fuel--    center          0.00000 ( 0.00000)              1348.5 (1967.6)      0.9682
                      fuel--                    0.08331 ( 0.03280)              1327.1 (1929.2)      0.9701
                      fuel--                    0.15618 ( 0.06149)              1274.6 (1834.6)      0.9750
                      fuel--                    0.21931 ( 0.08634)              1205.8 (1710.8)      0.9817
                      fuel--                    0.27339 ( 0.10763)              1131.9 (1577.8)      0.9893
                      fuel--                    0.31913 ( 0.12564)              1060.4 (1449.1)      0.9970
                      fuel--                    0.35724 ( 0.14064)               995.7 (1332.6)      1.0043
                      fuel--                    0.38841 ( 0.15292)               939.9 (1232.2)      1.0110
                      fuel--                    0.41336 ( 0.16274)               893.9 (1149.3)      1.0168
                      fuel--                    0.43278 ( 0.17039)               857.3 (1083.5)      1.0216
                      fuel--                    0.44738 ( 0.17613)               829.6 (1033.6)      1.0254
                      fuel--                    0.45783 ( 0.18025)               809.6 ( 997.5)      1.0282
                      fuel--                    0.46483 ( 0.18300)               796.1 ( 973.3)      1.0301
                      fuel--                    0.46908 ( 0.18468)               787.9 ( 958.5)      1.0313
                      fuel--                    0.47126 ( 0.18554)               783.7 ( 951.0)      1.0320
                      fuel--                    0.47207 ( 0.18585)               782.1 ( 948.2)      1.0324
                      fuel-- outer surface      0.47218 ( 0.18590)               781.9 ( 947.8)      1.0325

                      cladding inner surface    0.47942 ( 0.18875)               628.0 ( 670.8)
                      cladding outer surface    0.54691 ( 0.21532)               597.9 ( 616.6)

                      oxide surface             0.54692 ( 0.21532)               597.9 ( 616.5)

                      coolant temperature                                        573.3 ( 572.3)
```

D.2. FRAPCON-AM/MD BOL Radial Temperature Profile (node 4/12):

```
                    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
                    x                    **** FRAPCON-3.3 (Aug. 12 05) ****                    x
                    x                         Released August   2005                          x
                    x           Oconee rod 15309                                              x
                    x                  run date:  07-Oct-31           page    8                x
                    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

                                axial region number  5           power-time step   1

   avg.  linear heat rating, kW/m(kW/ft)    19.03(  5.80)
   local linear heat rating, kW/m(kW/ft)    23.70(  7.22)          rod surface heat flux, W/m**2(btu/hr-ft**2)
6.90E+05(2.19E+05)
   peak  linear heat rating, kW/m(kW/ft)    23.93(  7.29)

   step starts at time, days(sec)     0.00( 0.00E+00)              starting burnup,  MWd/kgU(MWd/mtU)    0.00(     0.)
   time increment,      days(sec)     0.10( 8.64E+03)              burnup increment, MWd/kgU(MWd/mtU)    0.00(     4.)
   end step,            days(sec)     0.10( 8.64E+03)              end step burnup,  MWd/kgU(MWd/mtU)    0.00(     4.)

                                          Radial temperature and power distribution

                                              Radii , cm(in)                Temperature, K(F)   Power profile

                          fuel--    center          0.00000 ( 0.00000)              1364.6 (1996.6)      0.9682
                          fuel--                    0.08332 ( 0.03280)              1339.8 (1951.9)      0.9701
                          fuel--                    0.15621 ( 0.06150)              1279.7 (1843.8)      0.9750
                          fuel--                    0.21934 ( 0.08635)              1203.3 (1706.3)      0.9817
                          fuel--                    0.27341 ( 0.10764)              1123.9 (1563.4)      0.9893
                          fuel--                    0.31915 ( 0.12565)              1049.7 (1429.7)      0.9970
                          fuel--                    0.35725 ( 0.14065)               984.5 (1312.5)      1.0043
                          fuel--                    0.38842 ( 0.15292)               929.9 (1214.2)      1.0110
                          fuel--                    0.41337 ( 0.16274)               885.9 (1135.0)      1.0168
                          fuel--                    0.43279 ( 0.17039)               851.6 (1073.3)      1.0216
                          fuel--                    0.44738 ( 0.17613)               826.0 (1027.0)      1.0254
                          fuel--                    0.45783 ( 0.18025)               807.6 ( 994.1)      1.0281
                          fuel--                    0.46483 ( 0.18301)               795.4 ( 972.1)      1.0301
                          fuel--                    0.46908 ( 0.18468)               788.0 ( 958.8)      1.0313
                          fuel--                    0.47126 ( 0.18554)               784.2 ( 952.0)      1.0320
                          fuel--                    0.47207 ( 0.18585)               782.8 ( 949.4)      1.0324
                          fuel-- outer surface      0.47218 ( 0.18590)               782.6 ( 949.1)      1.0325

                          cladding inner surface    0.47943 ( 0.18875)               630.6 ( 675.5)
                          cladding outer surface    0.54692 ( 0.21532)               600.9 ( 621.9)

                          oxide surface             0.54693 ( 0.21533)               600.8 ( 621.8)

                                  coolant temperature                                      576.6 ( 578.3)
```

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BIOGRAPHICAL SKETCH

Daniel Vega graduated from Franklin High School in El Paso, TX in 2000, and enrolled at Texas A&M University. While an undergraduate, Daniel studied physics and nuclear engineering, worked as a reactor operator at the Texas A&M Nuclear Science Center, and spent a year working on international nuclear safeguards for the International Atomic Energy Agency (IAEA) in Vienna, Austria. He graduated with a B.S. in nuclear engineering in December 2005, and pursued his maritime interests as a marine assistant on a National Science Foundation (NSF) funded marine geophysics cruise in Antarctica. Then, Mr. Vega enrolled as a graduate student at the University of Florida in the Department of Nuclear and Radiological Engineering, and has recently received an M.S. in nuclear engineering. He has accepted a position with the U.S. Department of Energy's Office of Nuclear Energy, and begins work in August 2008. His interests include outdoor activities, travel, music, and his dog, Sandwich.