DEVELOPMENT AND USE OF A HOMOGENIZED FUEL REGION MODEL FOR THERMAL ANALYSIS OF A TRUCK PACKAGE UNDER NORMAL AND FIRE ACCIDENT CONDITIONS

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ABSTRACT

In the current work, a geometrically-accurate two-dimensional model is developed of an isolated fuel assembly within isothermal compartment walls. Finite difference thermal simulations are performed to determine the cladding temperature for a range of compartment wall temperatures and assembly heat generation rates. The results for zero heat generation rate are used to determine a temperature-dependent effective thermal conductivity of the fuel region. The effective volumetric specific heat of the region is determined from a lumped capacity model. These effective properties are then applied to a two-dimensional model of a legal weight truck cask with homogenized (smeared) fuel regions. Steady-state normal conditions of transport simulations are performed for a range of fuel heat generation rates. The generation rate that brings the zircaloy cladding to their radial hydride formation temperature predicted by the homogenized model is greater than that determined by an accurate geometry model. Transient regulator fire accident simulations are performed for a range of fire durations. The minimum fire durations that bring the fuel cladding to its burst rupture temperatures are estimated. These results are compared to simulations which employ cask models with geometrically-accurate fuel region models.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tr>
<td>C</td>
<td>Conduction solution constant (Eqn. 4b)</td>
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<tr>
<td>c_v</td>
<td>Material specific heat at constant volume</td>
</tr>
<tr>
<td>c_v,E</td>
<td>Equivalent regional specific heat at constant volume</td>
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<tr>
<td>d</td>
<td>Fuel pellet diameter</td>
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<tr>
<td>D</td>
<td>Fire duration</td>
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<tr>
<td>D_c</td>
<td>Fire duration of concern based on cladding considerations</td>
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<td>H</td>
<td>Basket wall length</td>
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<td>k</td>
<td>Material thermal conductivity</td>
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<td>k_T</td>
<td>Effective thermal conductivity based on local temperature</td>
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<td>k_U</td>
<td>Effective uniform thermal conductivity</td>
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<tr>
<td>L</td>
<td>Active length of the assembly</td>
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<tr>
<td>q_AG</td>
<td>Pellet volumetric heat generation rate used in AG simulations</td>
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<td>q_HG</td>
<td>Fuel region volumetric heat generation rate used in HG simulations</td>
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<tr>
<td>Q</td>
<td>Total assembly heat generation rate [W]</td>
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<tr>
<td>Q_c</td>
<td>Total assembly heat generation rate limit based on cladding considerations</td>
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<tr>
<td>Q'</td>
<td>Assembly axial heat generation rate [W/m]</td>
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<tr>
<td>Q_c'</td>
<td>Assembly axial heat generation rate limit based on cladding considerations</td>
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<tr>
<td>N_G</td>
<td>Number of computational domain grid points</td>
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<tr>
<td>s</td>
<td>Cord coordinate (Figure 7)</td>
</tr>
<tr>
<td>t</td>
<td>Time after fire ignition</td>
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<tr>
<td>T</td>
<td>Local temperature</td>
</tr>
<tr>
<td>T_B</td>
<td>Boundary temperature</td>
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<tr>
<td>T_c</td>
<td>Maximum cladding or domain center temperature</td>
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<tr>
<td>T_CD</td>
<td>Cladding creep deformation temperature limit</td>
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<td>T_RH</td>
<td>Cladding radial hydride temperature limit</td>
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<td>T_BR</td>
<td>Cladding burst rupture temperature limit</td>
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<tr>
<td>T_PC</td>
<td>Peak Cladding Temperature</td>
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<tr>
<td>T_PCM   Maximum, post-fire peak cladding temperature</td>
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<tr>
<td>w</td>
<td>Radial coordinate (Fig. 3)</td>
</tr>
<tr>
<td>ε</td>
<td>Surface emissivity</td>
</tr>
<tr>
<td>ρ</td>
<td>Material density</td>
</tr>
<tr>
<td>ρ_E</td>
<td>Effective regional density</td>
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Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>AD</td>
<td>Angular Discretization</td>
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<tr>
<td>AG</td>
<td>Accurate Geometry</td>
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<td>BWR</td>
<td>Boiling Water Reactor</td>
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<td>CFD</td>
<td>Computational Fluid Dynamics</td>
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<td>ETC</td>
<td>Effective Thermal Conductivity</td>
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<td>HAC</td>
<td>Hypothetical Accident Conditions</td>
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<td>HG</td>
<td>Homogenized Geometry</td>
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<tr>
<td>He</td>
<td>Helium gas</td>
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<td>N_2</td>
<td>Nitrogen gas</td>
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<tr>
<td>NCT</td>
<td>Normal Conditions of Transport</td>
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<td>NRC</td>
<td>Nuclear Regulatory Commission</td>
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<tr>
<td>PWR</td>
<td>Pressurized Water Reactor</td>
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<tr>
<td>SAR</td>
<td>Safety Analysis Report</td>
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<tr>
<td>UNF</td>
<td>Used Nuclear Fuel</td>
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INTRODUCTION

Light water reactor nuclear fuel assemblies consist primarily of zircaloy cladding tubes filled with stacks of UO₂ fuel pellets [1]. The rods are held in square arrays by headers, footers and periodic spacer plates. Some positions in the array contain hollow instrumentation or guide thimble tubes instead of fuel rods. Different boiling water reactor (BWR) assemblies consist of 6×6 to 9×9 arrays of rods surrounded by a square-cross-section zircaloy channel. Pressurized water reactor (PWR) assemblies generally consist of 9×9 to 17×17 rod arrays but do not have surrounding channels.

After fuel is used in a reactor, the fuel pellets become highly radioactive, and radioactive fission gases are produced [2]. These used nuclear fuel (UNF) assemblies are stored underwater while their heat generation and radioactive decay rates decrease. After an appropriate time they are placed in packages for dry storage or offsite transport. In transportation, individual assemblies are supported horizontally within square cross-section basket openings inside the package containment region. That region is filled with helium (He), nitrogen (N₂), or another non-oxidizing cover gas. Packages transported by truck or rail have enough space for roughly 4 or 21 PWR assemblies, respectively [3,4].

Before a transport package may be used, its manufacturer must produce a safety analysis report (SAR) that demonstrates to the US Nuclear Regulatory Commission (NRC) that the package will maintain its shielding, criticality control, and containment functions during normal conditions of transport (NCT) and after a series of series of hypothetical accident conditions (HAC) [5]. This series includes a 9-m drop onto an unyielding surface, a 1- m drop onto a puncture bar, thirty-minutes in an 800°C, fully-engulfing fire, and water submersion.

The zircaloy cladding that encapsulates the fuel pellets provides an important confinement boundary that assures the fuel is in the configuration used in the SAR to analyze the package performance. The cladding integrity must therefore be protected. When fuel is transferred from underwater to dry storage, and during NCT, the fuel cladding may develop radial hydrides and become brittle if its temperature exceeds T<br > BR = 570°C or T<br > CD = 570°C or T<br > BR = 750°C [7].

Thermal finite element models are used to analyze transportation packages and determine their internal component and fuel cladding temperatures [3,4]. These models are subjected to different thermal boundary conditions to predict temperatures during NCT and HAC. Since packages are large and intricate, it is difficult and computationally intensive to explicitly model all the package components. For example, packages have multiple basket openings, each containing UNF assemblies submerged in gas. Moreover, each assembly contains hundreds of fuel rods. In the past computational resources were not available to model the fuel rods and gas separately. To address this problem, the fuel assemblies and cover gas were replaced homogenized solids with internal heat generation and effective thermal conductivities (ETC) [3, 8-11]. These ETCs were intended to model conduction and radiation heat transfer between the fuel and basket walls.

A shortcoming of these homogenized-geometry (HG) models with effective conductivities is that they approximate heat flux at a location based only on the temperature and its spatial gradient at that location. This may not be appropriate or accurate if radiation heat transfer is significant since its heat flux at a location depends on temperatures at a distance from that location. Moreover, natural convection heat flux is dependent on local velocity, which depends on temperatures at different locations. As a result, a conductivity model that is appropriate within fuel basket openings with nearly isothermal walls may not be accurate for openings where there is a large variation in the surface temperature.

Modern computational resources allow the use of two-dimensional package domains that accurately model the fuel and gas geometry in the multiple fuel regions. These accurate-geometry (AG) simulations have been used to predict cladding temperatures for NCT in rail [12] and truck [13] packages, designed to transport, respectively, 21 and 4 PWR assemblies. These AG meshes had 15×15 arrays of fuel rods in each basket opening. Computational fluid dynamics (CFD) simulations were used to calculate buoyancy-induced motion in, and natural convection and radiation heat transfer across, the cover gas. When He is the cover gas, the assembly heat generation rate that caused the cladding to reach the radial hydride formation temperature (T<br > RH = 400°C) was found to be 30% larger than when lower-conductivity N₂ is used. These results were effectively the same when buoyancy and natural convection in the gas was neglected.

Two and three-dimensional CFD simulations of natural convection and radiation heat transfer have been successfully benchmarked against steady state temperature measurements performed in horizontal and vertical arrays of heated rods inside gas-filled enclosures [14-19]. Those geometries represent UNF assemblies within basket openings.

Accurate-geometry transportation package simulations were also conducted for HAC in which a truck package containing four PWR assemblies was is exposed to an 800°C fire for different fire durations [20]. The minimum fire durations that cause the fuel cladding to reach the creep deformation or burst rupture temperatures (T<br > CD = 570°C or T<br > BR = 750°C) were determined, and found to decrease as the assembly heat generation rate increased. For a given assembly heat rate, the fire duration of concern was roughly the same for He or N₂ cover gas. This insensitivity to cover gas may be because, at the high fuel assembly temperatures caused by the fire, the rate of radiation heat transfer from the fuel rods to the basket walls was much greater than that transported by conduction in the cover gas. Another set of normal and accident condition simulations were performed with no gas motion. These stagnant-gas simulations, which required less computational resource than the ones that included motion, gave nearly the same fuel cladding temperatures. This indicates gas motion did not strongly affect the results and may not need to be modeled in some transport packages.

The objective of the current work is to evaluate the accuracy with which a two-dimensional package simulation that uses an
HG fuel region reproduces cladding temperatures predicted by an AG model, for both normal and fire accident conditions. To do this, an AG isolated fuel region model is constructed, consisting of a 15x15 array of fuel rods and cover gas within isothermal basket walls. Simulations are performed for a range of wall temperatures and rod heat generation rates. Those results are used to derive a temperature-dependent ETC for an HG fuel region that completely filled the basket cavity (there is no gap between the fuel block and the basket surfaces). This effective conductivity accurately reproduces the temperatures predicted in the AG fuel region model. The AG model of a truck package designed to transport four PWR assemblies, which was developed for earlier work [13, 20], was used to predict cladding temperatures under NCT with a range of fuel heat generation rates, and under HAC with different fire durations. The fuel region of that model was identical to the mesh used in the isolated fuel region model, but the basket temperature was calculated as part of the simulation (and not necessarily isothermal). The homogenized fuel region model was then implemented in the package model and used to predict the peak cladding temperature for NCT and HAC. The accuracy of the HG model in reproducing the AG results was then assessed.

In the HG simulations of the current work, each basket opening is completely filled with a solid with an ETC. This technique has been used in the SARs of some currently-licensed packages [3]. In contrast, in some package simulations, fuel blocks with an ETC are used to model fuel within each basket opening, and there is a gas-filled gap between the block and the basket surface [21,22]. A future extension of the current work may compare results from AG simulations with those that use gas-surrounded fuel block models.

ISOLATED FUEL REGION SIMULATIONS

Accurate Geometry (AG) Computational Model Figure 1 shows an accurate-geometry (AG) two-dimensional cross-section model of a General Electric (GE) 15x15 PWR fuel assembly [1] within a isolated square basket opening. This cross section consists of 225 10.9-mm-outer-diameter zircaloy cladding tubes with uranium dioxide (UO$_2$) fuel pellets of diameter d = 9.36 mm inside. In this model there is no gap or thermal contact resistance between the pellets and cladding. The rods are in a square array with 14.5 mm center-to-center pitch [10].

The basket surface is constructed from stainless steel and it is H = 217.5 mm on each side [3]. The assembly is centered within the opening. In different simulations either helium (He) or nitrogen (N$_2$) gas fills the space between the fuel rods and the basket.

Conduction is modeled within all solid and gas components of the model. The solid lines in Fig. 2 show the temperature-dependent thermal conductivity of the zircaloy cladding, UO$_2$ pellets, and He and N$_2$ gas used in this work [10]. It shows that the thermal conductivity of He is nearly an order of magnitude higher than that of N$_2$.

Surface-to-surface radiation is modeled across the gas. The emissivity of the zircaloy and stainless steel surfaces are, respectively, 0.806 and 0.6 [10]. Earlier work shows that natural convection does not strongly affect fuel clad temperatures within transport packages [12,13], so buoyancy induced gas motion is not included in this work. Future work may use a surface emissivity of 0.2 [3].

In GE 15x15 PWR fuel assemblies each rod contains a stack of fuel pellets with total length L = 3.601 m [1] in the direction normal to the plane of Fig. 1. Heat generation within the pellets varies with axial position and it peaks at an interior cross section. The peak axial fuel heat generation rate is

$$Q' = \frac{QP}{L},$$

where QP is the power per fuel pellet.
where \( Q \) is the assembly heat generation rate and the peaking factor \( P \) is the ratio of the maximum axial heat generation rate to the average value. For a used GE 15x15 PWR a representative peaking factor is \( P = 1.1351 \). In this work we calculate the temperature within the cross section with the maximum heat generation.

For the AG cross section in Fig. 1, the volumetric heat generation rate is uniform within all the fuel pellets and is calculated by dividing the axial heat generation rate by the area of the 225 fuel pellets within the cross section:

\[
q_{AG} = \frac{Q'}{225 \pi d^2}.
\]  

(2)

In this work the Fluent commercial CFD package is used to calculate conduction and radiation heat transfer and the resulting temperatures in the domain shown in Fig. 1. While Fluent has the capability to solve the momentum equation and calculate buoyancy induced gas motion, only stagnant gas simulations are performed in this work. Fluent uses the finite-volume method with second-order discretization. All simulations results presented in this work are from a mesh with \( N_G = 21,600 \) grid points and a surface-to-surface radiation angular discretization of \( AD = 6 \), unless otherwise stated. Simulations with two other mesh refinements \( N_G = 86,400, \) and \( 316,800, \) and four other angular discretizations \( AD = 2, 4, 8 \) and \( 10 \) were also performed. Those simulations showed that the results did not change substantially when \( N_G \) or \( AD \) increased above the values used in the simulations presented in this work.

The computational grid and material and surface properties are used to calculate the fuel temperature within the assembly cross section. These temperatures are calculated for different total fuel axial heat generation rates, \( Q' \), isothermal boundary temperatures \( T_B \), and for atmospheric-pressure He or \( N_2 \) cover gases.

**Accurate Geometry (AG) Simulation Results** Figure 3a shows temperature contours for the top right quadrant of the domain in Fig 1 for \( Q' = 166 \text{ W/m} \) (\( q_{AG} = 10,722 \text{ W/m}^3 \)), \( T_B = 25^\circ \text{C} \), and \( N_2 \) cover gas. For a typical GE 15x15 PWR assembly this peak axial heat generation rate corresponds to a total heat generation rate of 526W (using Equation 1 with \( L = 3.601 \text{ m} \), and \( P = 1.1351 \)). The highest temperature in this simulation is \( T_C = 87.3^\circ \text{C} \) and located at the bottom left corner of Fig. 3a, which represents the center of the assembly. The temperature decreases as the boundaries are approached (upper and right hand edges of Fig. 3a). The uneven texture in the contours is caused by the different conductivities in the gas and solid regions and the non-uniformity of the heat generation rate. The \( w \)-axis, whose origin is at the assembly center and which passes through the domain corner, is shown in Fig. 3.

In Fig. 4, the line marked AG shows the temperature \( T \) along the \( w \)-axis, minus the boundary temperature \( T_B \), versus location, for the same conditions as Fig. 3a. The temperature is relatively uniform in the rods compared to the temperature gradients that exist in the relatively low thermal conductivity gas. Two factors cause the temperature gradient to be steeper near the walls than it is near the assembly center. The first is that the radial heat flux increases as the walls are approached. The second is that radiation heat transfer is more important near the assembly center than it is near the boundaries because the center is hotter than the boundaries. The temperature difference between the fuel center and the boundary is \( T_C - T_B = 62.3^\circ \text{C} \).

The symbols in Fig. 5 show the maximum temperature difference within the domain, \( T_C - T_B \), versus assembly axial heat generation rate and boundary temperature. Figures 5a and 5b show results for nitrogen and helium cover gas, respectively. For a given boundary temperature these temperature differences increase with heat generation rate. The increase is not linear, especially for \( N_2 \) at higher heating rates, because the importance of radiation compared to conduction increases with temperature. The increased importance of radiation with temperature also

![Figure 3](image3.png)  
**Figure 3** Temperature contours within the upper right-hand quarter of the isolated fuel region model for \( N_2 \) with an isolated boundary temperature of \( T_B = 25^\circ \text{C} \) and fuel assembly heat generation rate \( Q' = 166 \text{ W/m} \) (a) Accurate Geometry (AG) simulation (b) Homogenized geometry (HG) simulation with a uniform effective conductivity \( k_U \)

![Figure 4](image4.png)  
**Figure 4** Temperature along \( w \)-axis shown in Fig. 3 minus boundary temperature versus distance from the fuel region center for an isolated fuel region for \( N_2 \), at \( T_B = 25^\circ \text{C} \) and \( Q' = 166 \text{ W/m} \). Results are shown for simulations using an accurate geometry (AG), and from homogenized geometry (HG) simulations using thermal conductivities that are uniform, \( k_U \), and temperature dependent, \( k_T \).
causes the temperature difference to decrease as the surface temperature increases. The temperature differences are also smaller for He than they are for N\textsubscript{2} because He has a much higher thermal conductivity.

Homogenized Geometry (HG) Computational Model

In this section we develop a "smeared" or homogenized-geometry (HG) model of a fuel assembly using effective thermal conductivities (ETC). The intent is for the model to calculate temperature profiles that approximate those predicted by AG models, but using less computational resources. This method is widely used in the nuclear industry to predict cladding temperatures within transport packages [23]. In HG models the heat is generated uniformly within the basket opening cross section, and an ETC, which depends only on the local temperature, is used to model the combined effects of conduction and radiation heat transfer.

To develop the HG model, we replace the accurate geometry in Fig. 1 with a solid that completely fills the area within the boundaries (as mentioned earlier, in this work there is no gap between the solid and the boundaries). For this model to generate heat uniformly and have the same axial assembly heat generation rate as the accurate-geometry one, the volumetric heat generation rate is

\[
q_{HG} = \frac{Q'}{H^2}.
\]  

(3)

As a first approximation we assume this region has a uniform thermal conductivity, k\textsubscript{U}, which \textit{does not} depend on the local temperature. For a square region with uniform conductivity and volumetric heat generation, and isothermal edges, the interior temperature may be calculated from a series solution of the Laplace heat conduction equation [24]. The temperature difference between the center of the square and its boundary is

\[
T_C - T_B = C \frac{Q'}{k_U},
\]  

(4a)

where C is a constant evaluated as

\[
C = \frac{1}{8} - 4 \sum_{n=0}^{\infty} \left[ (-1)^n \left( \frac{\pi^2}{4n^2+1} \right)^3 \cosh \left( \frac{\pi}{2n+1} \right) \right] = 0.07395.
\]  

(4b)

Equation 4a can be rearranged to calculate the equivalent uniform-conductivity that gives the same maximum temperature difference (T\textsubscript{C} - T\textsubscript{B}) as the heterogeneous AG model,

\[
k_U = C \frac{Q'}{T_C - T_B}.
\]  

(5)

For the simulation in Fig. 3a with Q' = 166 W/m, T\textsubscript{B} - T\textsubscript{C} = 62.3ºC, equation 5 gives the equivalent uniform conductivity 0.196 W/mK.

An HG simulation was performed using this uniform conductivity, a uniform heat generation rate of q\textsubscript{HG} = 3509 W/m\textsuperscript{3} (corresponding to Q' = 166 W/m) and T\textsubscript{B} = 25ºC. Figure 3b shows the resulting temperature contours in the upper right-hand quadrant of the domain. Like the contours in Fig. 3a, the maximum temperature is at the domain center (bottom left corner of Fig. 3b) and equal to T\textsubscript{C} = 87.3ºC, and the temperature decreases as the domain edges are approached. However, since this simulation uses uniform heat generation and thermal conductivity, the contour texture is more regular than it is in Fig. 3a.

The temperature along the w-axis in Fig. 3b, minus the wall temperature, is plotted in Fig. 4 and marked HG-k\textsubscript{U}. The temperature-difference is exactly the same as it is for the accurate geometry simulation at w = 0 and at the domain boundary. However, between those locations the uniform conductivity simulation gives a smoother temperature profile. That profile is systematically below the accurate-grid simulation results at most all locations. This difference is caused by the effects of radiation heat transfer. In the AG simulation, the
radiant heat flux across the gas is larger relative to conduction near the center of the domain, where the temperature is greater, than it is at the edge, where the temperatures are lower. For the HG simulation to be more physically accurate the effective-conductivity needs to increase with temperature so that it will better model the effect of radiation. However, the uniform conductivity $k_U$ is independent of local temperature.

In general the uniform conductivity $k_U$ can depend on $T_B$, $Q'$, and cover gas composition. This is because those quantities affect the temperatures within the domain, and the relative importance of conduction and radiation. The AG temperature differences (symbols) in Fig. 5 are used in Eqn. 5 to determine $k_U$ versus $Q'$ and $T_B$, for the geometry and material properties of the AG model. These results are shown in Figs. 6a and 6b for $N_2$ and He, respectively. This data confirms that $k_U$ is a function of $Q'$, $T_B$, and the cover gas, that is $k_U(T_B, Q, \text{gas})$.

Results in Fig. 6 are plotted for both positive and negative values of $Q'$, which correspond to heat generation and absorption within the fuel pellets (the heat absorbing simulations are physically relevant for spent fuel packages but were performed to allow $k_U$ to be interpolated for $Q' = 0$). Figure 6 shows that $k_U$ increases with $T_B$ and $Q'$ since the effect of radiation increases with temperature. At moderately low boundary temperatures ($T_B \leq 400°C$) the effective conductivity is higher when He is the fill gas, than that for $N_2$ due to helium’s higher thermal conductivity. At the highest boundary temperatures, however, the effective conductivities are nearly the same for both gases. This is because the fraction of heat transferred by conduction compared to radiation is very small at high temperatures. This makes the effective conductivity at high temperature essentially independent of gas conductivity.

**HG Effective Conductivity** We wish to develop effective thermal conductivities, which depend only on the local temperature $T$ and gas ($N_2$ or He), that is $k_{U,\text{gas}}(T)$, that may be used in an HG domain. These conductivities must have three important characteristics. The first is that they reproduce the AG profile (like the one in Fig. 4) more accurately than the HG-$k_U$ simulation. The second is that it will reproduce the AG maximum temperature difference versus $Q'$ and $T_B$ results shown in Fig. 5 (symbols). Lastly, they must be appropriate for temperatures between 38°C and 750°C. The lower temperature limit is NCT environment temperature, and is the lowest temperature the fuel may experience. The upper limit is the temperature at which the fuel cladding may experience burst rupture, and is the highest fuel temperature that must be analyzed.

Figure 6 shows that $k_U$ depends on $T_B$, $Q'$, and gas composition. We would like to find an appropriate temperature to associate with each value of $k_U$, but for each simulation the temperature within the domain varies between $T_B$ and $T_C$. The only condition under which the domain temperature is uniform ($T_B = T_C$) is for $Q' = 0$. For a given boundary $T_B$, the data in Fig. 6 can be interpolated to find a value of $k_U$ at $Q' = 0$. We also note that when $Q' = 0$, the entire domain is at the boundary temperature. In this work the temperature-dependent effective conductivity $k_{U,\text{gas}}(T)$ is determined from the uniform conductivity $k_U(Q', T_B, \text{gas})$, as:

$$k_{U,\text{gas}}(T, \text{gas}) = k_U(Q' = 0, T = T_B, \text{gas}).$$  \hspace{1cm} (6)
surface-to-surface radiation compared to conduction increases with temperature, making the gas conductivities less important.

An HG simulation that uses the temperature-dependent effective conductivity for N\textsubscript{2} with Q\textsuperscript{'} = 166 W/m and T\textsubscript{B} = 25°C produces temperature contours that are similar looking to those in Fig. 3b. The temperature difference along the w-axis for that simulation is shown in Fig. 4, using the line marked HG-k\textsubscript{T}. That contour more closely follows the accurate grid simulation result than the one from the HG-k\textsubscript{U} calculation. The solid lines in Figs. 5a and 5b show the center-to-boundary temperature difference versus Q\textsuperscript{'} and T\textsubscript{B} using HG simulations with the ETCs for He and N\textsubscript{2} cover gases. The values of T\textsubscript{C}–T\textsubscript{B} predicted by these HG simulations are systematically lower than those predicted by the AG simulations (symbols), and the difference increases as Q\textsuperscript{'} increases and as T\textsubscript{B} decreases. However, these differences are less than 0.9°C for all conditions shown in Fig. 5.

The temperature-dependent ETCs in Equations 7a and 7b are used in HG simulations in the remainder of this work.

FULL PACKAGE SIMULATIONS

Computational Model Figure 7 shows the two-dimensional finite-element model of a legal-weight-truck package that the current authors used in earlier geometrically-accurate simulations [13, 20]. This model is similar but not identical to the cross section of a package that is currently-certified to transport 4 PWR assemblies [3]. Only half of the package is modeled to take advantage of its symmetry.

The model contains two fuel regions whose characteristics are identical to those in Fig. 1 (future work may consider a basket emissivity of 0.2, which is the value associated with the currently-licensed package [3]). These fuel regions are surrounded by a 0.96-cm-thick stainless steel liner. The liner is surrounded by a 6.7-cm-thick depleted uranium gamma shield. Outside of this shield are a 3.8-cm-thick stainless steel package body, a 12.1-cm thick polypropylene-1% boron neutron shield, and a 0.27-cm-thick stainless steel skin. The thermal conductivities used in this work for the depleted uranium and polypropylene-1% boron, are constant and equal to, respectively, 25.49 W/mK, and 5 W/mK. For stainless steel, the conductivity is 10.8 W/mK and 19.1 W/mK, at temperatures of 4°C and 504°C, and varies approximately linearly in between. At higher temperatures the conductivity in this model is 19.1 W/mK. Future work may include more realistic temperature-dependent conductivity properties for these materials.

Figure 7 shows the s-coordinate system. Its origin is at the lower left hand corner of the upper fuel region. It follows the basket surface, first upward to the top of the opening, and then along the top to the outer corner.

In this paper we perform AG simulations in which separate regions are used for the fuel, cladding and gas. We also perform HG simulations in which all of the elements within the fuel regions are assigned the temperature-dependent ETCs from either Equations 7a or 7b for He or N\textsubscript{2} cover gases, respectively. In the AG model heat is generated within the fuel pellets only, while it is generated uniformly within the basket walls in the HG model. For a given assembly axial heat generation rate Q\textsuperscript{'} the volumetric heat generation rates for the AG and HG models, q\textsubscript{AG} and q\textsubscript{HG}, are calculated using Equations 2 and 3, respectively.

Coarse and fine computational meshes, with N\textsubscript{G} = 46,798 and 210,874 nodes, were used to evaluate the dependence of the results on the mesh refinement. Unless stated otherwise, all full package simulation results in this paper are from the 46,798-node model. All full package AG simulations used an angular discretization of AD = 6. The fuel regions of the smaller full-package mesh are identical to the coarse (21,600 node) isolated fuel region model described earlier. While isothermal boundary conditions were applied to the isolated fuel region model, the temperature of the fuel region boundaries within the full package model are determined as part of the simulation.

Normal Conditions of Transport Results Steady-state simulations are performed with the package in an NCT thermal environment [5], consisting of still air at 38°C, and a solar heat flux of 388 W/m\textsuperscript{2}. Heat generated by the fuel within the package and solar heat flux absorbed by its surface are
ultimately dissipated to the environment by natural convection and radiation heat transfer. The NCT natural convection heat transfer coefficient is based on the Churchill and Chu correlation [25], and the external surface radiative emissivity used in this work is 0.2 [3].

Figures 8a and 8b show the temperature contours within the package model from AG and HG simulations under NCT for an assembly axial heat generation rate of $Q' = 750 \, \text{W/m}$ (for each assembly), and $N_2$ cover gas. For a typical GE 15x15 PWR assembly this peak axial heat generation rate corresponds to a total heat generation rate of 2379 W. Both simulations were performed using the same $N_2 = 46,798$ grid point mesh. In the HG simulation $k_{T,N2}(T)$ and $q_{HG}$ were assigned to all the grids points within the fuel regions, while in the AG model, the actual material properties and $q_{AG}$ were assigned to the appropriate nodes.

The contours from the two simulations are similar, especially outside of the fuel regions. Within the fuel regions the contours from the homogenized-geometry simulation are smoother than those from the accurate-geometry calculation. The minimum package surface temperature from both simulations is 139°C, which is roughly 100°C hotter than the NCT surroundings. This temperature difference is strongly affected by the external package natural convection coefficient and radiation heat emissivity. Uncertainty in these quantities has a strong effect on the predicted package surface and peak cladding temperature. As a result, future work should investigate the accuracy of the package external surface heat transfer calculations.

The maximum cladding temperatures from the AG model is 362°C, and the maximum fuel region temperature from the HG model is 350°C. Both of these temperatures are below the allowed value of 400°C for NCT [6]. However, these predicted temperatures differ by 12°C. In contrast, for the isolated fuel region simulations, the maximum difference between peak fuel region temperature predicted by AG and HG simulations was always less than 0.9°C.

To understand why the difference between the peak temperatures from the AG and HG simulations are greater for the full-package model than they are for the isolated fuel regions we must consider the fuel region boundary temperatures. Figure 9 shows the basket surface temperature versus the s-coordinate (described in Fig. 7) divided by the wall length, $s/H$. Results are shown for $Q' = 750 \, \text{W/m}$ for both AG and HG simulations and $N_2$ and He cover gases. For each simulation, the hottest and coolest surface temperatures are near the inside and outside corners of the opening (near $s/H = 0$ and 2). The temperature decreases significantly with distance from the package center along the wall that radiates from the package center ($0 \leq s/H \leq 1$). The temperature is much more uniform along the edge near the package outer boundary ($1 \leq s/H \leq 2$). For all four simulations the outside corner temperature is roughly 174°C, but the inside corner is between 183°C and 129°C warmer.

The ETCs in Equations 7a and 7b were derived so that HG models accurately reproduced the temperature profiles and maximum temperature calculated by AG models in fuel region models with isothermal boundaries. However in a full package model, whose basket surface temperature is strongly dependent on location, the HG simulations predict lower fuel region temperatures than the AG calculations. As mentioned earlier, when radiation heat transfer is significant, the heat flux at each location within the fuel region depends on temperatures at a distance from that location. However, homogenized models that employ effective thermal conductivities approximate the heat flux at a location based solely on the temperature and its special gradient at that location.

Figure 10 shows the peak fuel region temperature from HG simulations and the peak cladding temperature from AG calculations versus assembly axial heat generation rate with He and $N_2$ cover gases. For the heat generation rates used in this figure, the calculated temperatures are higher when $N_2$ is the cover gas than it is for He, due to $N_2$’s lower thermal conductivity. For each gas, the AG calculations consistently predict higher temperatures than the HG simulations (due to the
non-uniform basket surface temperatures). A horizontal line in Fig. 10 marked $T_{RH} = 400^\circ$C shows the maximum allowed fuel clad temperature during normal conditions of transport [6]. The maximum allowable axial heat generation rate based on cladding consideration, $Q_C$, is the value that causes the cladding to reach this allowed temperature. Table 1 summarizes the values of $Q_C$ calculated for both gases and both simulation methods. The values in parentheses are the corresponding allowable total assembly heat generation rates $Q_C$ for typical 15x15 GE PWR fuel.

The AG simulations indicate that the allowable assembly heat generation rate is 25% higher when He is the cover gas than when lower-conductivity $N_2$ is used. HG simulations predict higher allowable heat generation rates than the AG calculations. The HG allowable heat generation rates are higher by 2.8% for He and 5.0% for $N_2$. These differences are relatively small. However, if the heat generation rates predicted by the HG model were used, the AG model, from which the HG model was derived, would predict that the cladding temperatures would exceed their allowed temperatures. The HG model described in this paper would therefore not be considered a conservative method to reproduce the temperatures calculated using AG simulations.

Other investigators may develop ETCs using different methods than the ones derived in the current paper. For example, some fuel region models employ a gas-filled gap between the fuel block and the basket. These other models may more accurately or conservatively reproduce the peak cladding temperatures predicted by the AG models from which they are derived. However, we are not aware of any other work in the open literature in which the results of HG full package simulation results are compared to AG full package results from which they were derived. The current work indicates there is a possibility that full package HG simulations may not always be conservative. We note, however, that comparing one numerical model to another has shortcomings compared to evaluating numerical results using experimentally measured temperatures in an actual transport package.

<table>
<thead>
<tr>
<th>Cover Gas</th>
<th>$Q'_C$ [W/m-assembly]</th>
<th>$Q_C$ [W/assembly]</th>
</tr>
</thead>
<tbody>
<tr>
<td>AG</td>
<td></td>
<td></td>
</tr>
<tr>
<td>He</td>
<td>1139 (3613)</td>
<td></td>
</tr>
<tr>
<td>$N_2$</td>
<td>909 (2884)</td>
<td></td>
</tr>
<tr>
<td>HG</td>
<td>1172 (3718)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>954 (3026)</td>
<td></td>
</tr>
</tbody>
</table>

**Hypothetical Fire Accident Results** Transient (time-dependent) simulations are performed to determine the package response to a hypothetical fire. NCT simulation results are used as the package initial condition before the fire. During the fire, the package surface emissivity is set to 0.8, and its environment temperature and emissivity are set to 800°C and 0.9, respectively. Simulations are performed for the regulatory fire duration of $D = 0.5$ hour, and for a range of longer lasting fires. After the simulated fire is extinguished at $t = D$, the environment is returned to NCT.

The specific heat at constant volume $c_v$ and density $\rho$ of each package material or region is required for transient calculations. In this work constant (not temperature dependent) values are used for all the materials. Table 2 summarizes the values of $\rho$, $c_v$, and the cross sectional area $A$ (volume per unit length normal to the page of Fig. 1) for each material within the fuel region. These properties are used in the AG simulations. The effective volumetric specific heat $c_{vE}$ and density $\rho_E$ of the homogenized fuel region are calculated as

$$\rho_E = \frac{\sum_i \rho_i A_i}{\sum_i A_i} , \text{ and}$$

$$c_{vE} = \frac{\sum_i \rho_i c_{vi} A_i}{\sum_i \rho_i A_i} .$$

These effective values are given in Table 2. They are nearly the same when He or $N_2$ is the cover gas.

Outside of the fuel region, the specific heats used in this work for the stainless steel, depleted uranium, and polypropylene-1%-boron are, respectively, 548 J/kgK, 133
J/kgK, and 927 J/kgK, while their respective densities are 7826 kg/m$^3$, 19,140 kg/m$^3$, and 2691 kg/m$^3$. While the polypropylene-1%-boron is expected to melt or react at elevated temperatures, these changes are not included in the current paper. Future work may include more realistic temperature-dependent properties for these materials.

Figure 11 shows the peak fuel temperature versus time during and after a regulatory fire of duration $D = 0.5$ hour. A vertical dash-dot line shows the end of the fire and beginning of the post-fire period. The solid lines shows the peak cladding temperature from AG simulations and the dashed lines show the peak fuel region temperature from HG calculations. Results are presented for both He and N$_2$ cover gases. For each simulation the fuel axial heat generation rate was set to $Q' = Q_C$ (from Table 1), which causes the initial peak clad temperature to be 400°C.

Figure 11 shows that the peak fuel temperature does not exhibit a significant rise until several minutes after the fire is out. The cladding temperature increases after the fire is extinguished because heat from the hotter outer portions of the package continues to diffuse toward the package center for a period of time.

The maximum peak cladding temperature, $T_{PC,M}$, is the highest cladding temperature caused by the fire. The AG simulations indicate that when N$_2$ is the cover gas $T_{PC,M} = 433°C$, and occurs at $t = 6.6$ hr. When He is the cover gas $T_{PC,M}$ is 8°C hotter and occurs 0.7 hours sooner.

To understand this temperature difference, we consider the axial heat generation rate used in each simulation. Table 1 shows that $Q'_{C}$ is greater in packages that use He as the cover gas than it is for packages that use N$_2$ (due to He’s higher conductivity). However, at the high temperatures the fuel reaches during the fire, radiation heat transfer becomes more dominant, and the relative heat transfer advantage He had due to its higher conductivity decreases. Since the He-filled package uses a higher assembly heat generation rate than the N$_2$-filled package, fuel in the He-filled package experiences higher temperatures after the fire.

The HG simulations predict cooler values of $T_{PC}$ during the first four hours after the fire is ignited, but cooler temperatures thereafter. They predict values of $T_{PC,M}$ that are 1°C to 2°C warmer, and occur 8 to 12 minutes later than those predicted by AG simulations. Because the HG model predicts higher temperatures, it is conservative compared to the AG model with regard to predicting if the cladding will exceed its allowed temperature. For both cover gases and fuel models, $T_{PC,M}$ is well below the values that may cause creep deformation or burst rupture of the cladding.

Figure 12 shows the peak clad temperature versus time during a long lasting fire where $D = 30$ hr fire. The solid lines shows the peak cladding temperature from AG simulations and the dashed ones show the peak fuel region temperature from HG calculations. Results are presented for both He and N$_2$ cover gases. Similar to Fig. 11, the axial heat generation rates used in these simulations cause the initial peak cladding temperature to be 400°C. Horizontal lines show the temperatures at which fuel cladding may exhibit creep deformation, $T_{CD} = 570°C$, or burst rupture, $T_{BR} = 750°C$.

During the long lasting fire, the peak fuel temperature is higher when He is the cover gas than when N$_2$ is used. This is
the same as for the D = 30 minute fire described earlier. Careful examination of the data shows that during the first two hours of the fire, when the fuel temperatures are relatively low, the AG simulations predict higher T_{PC} than the HG simulations. However, after that time the HG simulations predict higher temperatures than the AG calculations.

The AG simulations indicate T_{PC} will reach T_{HR} at t = 8.3 or 9.1 hour, respectively, when He or N\textsubscript{2} cover gases are used. The HG simulations predict T_{PC} will reach this temperature roughly 0.25 hours sooner. In this paper the fire duration of concern based on cladding temperature, D\textsubscript{C}, is the minimum fire duration that has the potential to cause the cladding temperature to reach T_{PC}. Since the cladding temperature generally increases for a period of time after the fire is extinguished, D\textsubscript{C} predicted for each cover gas and fuel region model will be slightly shorter than the times when the T_{PC} curves in Figure 12 cross the T_{PR}. Future work will estimate D\textsubscript{C}, for a range of Q'.

SUMMARY

A two-dimensional accurate-geometry (AG) model of an isolated, used 15x15 pressurized water reactor assembly within a basket opening of a transport package was constructed. The model was used in thermal simulations to predict the peak cladding temperature for ranges of fuel axial heat generation rates, isothermal boundary temperatures, and for both helium (He) and nitrogen (N\textsubscript{2}) cover gases. These results were used to develop different temperature-dependent effective fuel region thermal conductivities for He-filled and N\textsubscript{2}-filled packages. These conductivities were implemented in a homogenized-geometry (HG), or smeared, fuel region solid model. This model accurately reproduced the AG peak cladding temperatures for a relevant range of fuel heat generation rates, isothermal boundary temperatures, and with He and N\textsubscript{2} cover gas.

A two-dimensional AG model of a truck package was then used to predict the peak cladding temperature during normal conditions of transport (NCT) for a range of fuel axial heat generation rates, and for both He and N\textsubscript{2} cover gases. These simulations showed that the actual fuel region boundary temperatures were highly non-uniform. The fuel region was then replaced by a HG heat generating solid that employed the temperature-dependent effective conductivities developed earlier in this work. The peak cladding temperatures predicted by the HG package model were systematically lower than those predicted by the AG model for the full range of fuel heat generation rates examined, and for both He and N\textsubscript{2} cover gases. The HG model would therefore not be considered a conservative approximation of the AG-predicted temperatures, because it over-predicts the heat generation rate that causes the cladding to reach its allowed limit temperature.

The NCT simulation results were used to predict the peak cladding temperature versus time during and after regulatory format fires. Simulations were performed for He-filled and N\textsubscript{2}-filled packages, using both AG and HG computational models. In each simulation, the fuel axial heat generation rate was set to the value that caused the NCT peak cladding temperature to be 400°C. The simulated fire caused the fuel in He-filled packages to reach higher temperatures than in N\textsubscript{2}-filled packages. This is because a higher heat generation rate was used in the He-filled package, and at the high temperatures relevant during the fire the higher conductivity of the He gas does not significantly increase the heat transfer beyond that of radiation. The HG model predicted higher temperatures than the AG model. The HG model would therefore be a conservative approximation of the AG model under these conditions.

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REFERENCES


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