SIMULATE5 FUEL PIN MODEL DESCRIPTION AND VERIFICATION AGAINST ENIGMA

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ABSTRACT

SIMULATE5 is Studsvik's next generation nodal code [1]. One of SIMULATE5's novel features is a simplified fuel pin model that calculates the nodal fuel temperatures for the evaluation of the Doppler feedback. The purpose of this paper is twofold: (1) provides a description of SIMULATE5 fuel pin model and (2) presents the results of the verification against the fuel performance code ENIGMA [2]. Eighteen PWR rods and twenty-four BWR rods of different design were analyzed in the burnup range 0 to 60 MWd/kgU. They cover most of the historical and the present designs. To assess the SIMULATE5 fuel pin model, the chosen figure of merit was the volume-averaged fuel temperature because it is used in the evaluation of the Doppler feedback. For each of the forty-two rods, over the burnup interval 0-60 MWd/kgU, the differences between the SIMULATE5 and the ENIGMA volume-averaged fuel temperatures were evaluated. For the PWR rods, on average, SIMULATE5 predicts volume-averaged fuel temperatures that differ between -4K to +20K with respect to ENIGMA. For BWR rods, the differences are between -10K to +10K.

1. Introduction

SIMULATE5 [1], Studsvik's next generation nodal code, has been developed to address the challenges of advanced core designs with increased heterogeneity and aggressive operating strategies. SIMULATE5 relies on detailed modeling of the fuel assembly geometry considering the complicated mix of fuel enrichment zones, control rod zones, and spacer grids. The 3D fuel temperature distribution is evaluated in the channel thermal-hydraulic module by solving the one-dimensional, radial heat conduction equation for the average fuel pin of each node instead of relying on pre-computed fuel temperature tables. The purpose of this paper is twofold: (1) in Section 2, provides a description of the simplified fuel pin model and (2) in Section 3 provides the verification of the volume-averaged fuel temperature (TFU) computed by SIMULATE5 against the reference solution provided by the well-known fuel performance code ENIGMA developed by National Nuclear Laboratory in the United Kingdom [2]. Finally, some conclusions are drawn in Section 4.

2. Model description

An average fuel rod provides the feedback between SIMULATE5 neutronic and channel thermal-hydraulic models. The volume-averaged fuel temperature is used to evaluate the cross-sections, and the heat transferred to the coolant provides the hydraulic feedback. The rods are divided into regions: fuel pellet, gap and cladding as shown in Fig. 1.

The heat conduction in the fuel rod is governed by the one-dimensional, radial heat conduction equation. The thermal properties are considered functions of the local temperatures and the material composition of the different regions in the fuel rod (i.e. fuel pellet, gap and cladding). Descriptions of the treatment, the fuel thermal conductivity, the pellet-cladding gap model and the heat source are provided in what follows.
2.1 Fuel thermal conductivity

The fuel thermal conductivity depends on the fuel type composition (i.e. UO₂ or MOX), burnup and temperature. The modified Nuclear Fuel Industries (NFI) correlation for Urania pellets and the Duriez-modified NFI correlation for MOX pellets - as described in reference [4] - have been implemented in SIMULATE5. There is no explicit dependence on the Pu content for MOX fuel.

The fuel pellets are divided into a series of rings (typically 10), and the thermal conductivity is computed for each ring. The ring local temperature, and burnup are used for the evaluation of the thermal conductivity. The ring local burnup is evaluated using the nodal burnup and the intra-pellet radial burnup profiles pre-computed with CASMO5 [5] as described in Section 2.3 below.

The changes in the local density with burnup are neglected in this model; that is the as-fabricated pellet density is used to correct the fuel thermal conductivity computed using the NFI correlations. However, a simple correction to the as-fabricated pellet fuel density is introduced to simulate, to some extent, the rim effect at high burnup (> 40 MWd/kgU). The correction to the as-fabricated density is a quadratic function of the average burnup in excess of 40 MWd/kgU.

2.2 Fuel-cladding gap thermal conductance

The gap thermal conductance is the sum of three components: the gaseous conductance through areas of non-contact, the solid contact conductance through contact areas, and the radiation heat transfer from the fuel surface. The gap gaseous conductance governs the heat transfer from BOL (when the gap is open) until gap closure. The solid contact conductance governs the heat transfer after gap closure. The radiation heat transfer from the fuel surface is negligible in normal operating conditions and is not modelled in SIMULATE5.

The gaseous conductance models the following physical effects: fuel pellets irradiation swelling and densification, fuel pellets and clad thermal expansion, clad compression caused by irradiation at high pressure (clad creep-down), and the gas thermal conductivity degradation as the result of fission gas release. The gaseous conductance may be expressed as follows [6],

\[ h_g = \frac{k_g(1-\xi)}{g+g_0+g_3} + \frac{k_g\xi}{g_0+g_3} \]

Eq. 1

\( k_g \) is the modified thermal conductivity for the gas, \( \xi \) is the fraction of the fuel-cladding interface in solid contact, \( g \) is the average radial gap, \( g_0 \) is the temperature jump distance for the gas and \( g_3 \) is the fragmented fuel roughness. The SIMULATE5 fuel pin model does not explicitly treat the fission gas release during the life of the fuel. Instead, it assumes that the gap is initially filled with helium, and a degradation factor, as a function of burnup, models the change of the thermal conductivity due to fission gases. The Kjaerheim-Roldstad model [6] expresses the relationship between the fraction of fuel-cladding interface in solid contact and the average radial gap,
\[ \xi = C_2 \frac{100 \cdot g}{r_f} \]  
Eq. 2

\( C_2 \) is a model constant and \( r_f \) is the fuel pellet radius. Finally, the average radial gap dimension is given by,

\[ g = r_{cl} - r_{fp} \]  
Eq. 3

\( r_{fp} \) is the effective fuel pellet radius corrected for thermal expansion, densification and swelling, and \( r_{cl} \) is the effective cladding radius corrected for creep-down and thermal expansion.

The contact conductance between two solids (fuel pellets and cladding) is a function of, among other quantities, the thermal conductivities of the two materials and the contact pressure between them. The calculation of contact pressure would require the solution of the strain and stress fields for the whole rod. Instead, the contact conductance is approximated as a function of the solid contact fraction, such that the contact conductance is negligible when the gap is open (\( \xi \approx 0 \)) and significant when the gap closes (\( \xi \approx 1 \)).

### 2.3 Heat source – Intra-pellet power and burnup distributions

The spatial distribution of the volumetric heat source is dependent on the fuel burnup. The intra-pellet radial power and burnup profiles, as a function of the average burnup, have been pre-computed for UO\(_2\) and MOX with CASMO5 [3] and tabulated for ten radial rings over the burnup range from 0 to 70 MWd/kg\( U \). The 70 MWd/kg\( U \) intra-pellet profiles are used if the average burnup is greater than 70 MWd/kg\( U \). Fig. 2 provides the intra-pellet power profiles for typical UO\(_2\) and MOX pellets at 3 different burnup levels (0, 30, and 60 MWd/kg\( U \)).

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**Fig. 2** Intra-pellet power profiles UO\(_2\) and MOX at 0, 30, and 60 MWd/kg\( U \)
Four PWR rod geometries (14×14, 15×15, 16×16, and 17×17), and five BWR rod geometries (7×7, 8×8, 9×9, 10×10 SVEA and 10×10 GE) were analysed with CASMO5. Average core conditions were assumed in the pin-cell calculations, for example all BWR cases have a 40% void and all the PWR cases have a boron concentration of 800 ppm. Two fuel types were investigated: (1) a reactor grade UO₂ fuel, enrichment 4.5%, density 10.4 g/cm³; and (2) a reactor grade MOX fuel, 5 wt.% PuO₂. For practical purposes, the BWR cases were run with UO₂ fuel only. Therefore, a total of 13 depletion cases were considered: 4 PWR UO₂, 5 BWR UO₂, and 4 PWR MOX. Although PWR and BWR pin cells have totally different conditions, the intra-power shape difference between a PWR UO₂ and a BWR UO₂ pin cell is small. The maximum root mean square (RMS) differences for all burnups is lower than 0.8%. Therefore, it is not necessary to differentiate between PWR and BWR in terms of the intra-pellet radial power distribution, one set of data suffices. However, the MOX and UO₂ PWR rods are different. At BOL, the power shape RMS difference is 5.5%. As burnup proceeds, the RMS difference gradually decreases. In summary, as shown in Fig. 2, two sets of intra-pellet power distributions are adequate for the SIMULATE5 fuel pin model, i.e., a UO₂ data set and a MOX data set.

3. Verification

The figure of merit to evaluate the quality of the SIMULATE5 solution is the volume-averaged fuel temperature (TFU), because it is used in the cross-sections evaluation (i.e. the Doppler feedback). The fuel rods analysed in what follows were taken from available SIMULATE5 core models. This selection imposes limitations with regards to the rod characteristics and their operating conditions.

Section 3.1 and Section 3.2 compare the TFU computed by SIMULATE5 and the fuel performance code ENIGMA for the PWR and the BWR environment respectively.

3.1 PWR environment

Eighteen PWR rods of different design were modelled using SIMULATE5 and ENIGMA. The cases cover many of the present PWR designs (14×14, 15×15, 16×16, and 17×17 geometries); the initial cold radial gap is between 75 and 110 microns; the nominal power is between 10 kW/m and 23 kW/m; and the rod internal pressure is between 1.7 MPa and 3.1 MPa.

Fig. 3 compares the rise of the TFU above the coolant temperature as a function of burnup at nominal conditions for a 17x17 rod and a 16x16 rod. The red line represents the ENIGMA reference solution, the blue line represents the SIMULATE5 solution and the green line the differences (SIMULATE5 minus ENIGMA).

![Fig. 3 Fuel average temperature above coolant temperature for two typical PWR rods](image-url)
Results for all PWR rods are summarized in Fig. 4 and Fig. 5. Fig. 4-a through Fig. 4-c show the TFU differences with respect to the ENIGMA reference solution at 0 MWd/kgU (rod BOL), 20 MWd/kgU (representative of the burnup at which the fuel-clad gap closes), and 60 MWd/kgU (representative of an average fuel rod EOL) respectively.

Fig. 4-d shows the TFU differences as a function of the nominal linear heat generation rate (LHGR) at three different burnups: 0 MWd/kgU, 20 MWd/kgU, and 60 MWd/kgU. Note that there is no strong dependence of the TFU differences with the nominal LHGR. This fact gives us confidence that the limited LHGR range does not invalidate the conclusions of this study.

Fig. 4  Averaged fuel temperature differences for all PWR rods at three different burnups

Fig. 5 summarizes for each of the eighteen PWR rods, the maximum, average and minimum TFU differences in the burnup range 0 to 60 MWd/kgU.
From the figures above, the following observations can be made:

- At BOL (0 MWd/kgU): the agreement between the present solution and the ENIGMA reference solution is good. Differences are within ±10 K (see Fig. 4-a).

- After one cycle of irradiation (represented by the 20 MWd/kgU data): The differences are between -10 K and +40K with respect to the ENIGMA reference solution (see Fig. 4-b).

- At EOL (represented by the 60 MWd/kgU data): The SIMULATE5 solution differs between +0 K and +12 K with respect to the ENIGMA reference solution (see Fig. 4-c).

- In the examined burnup range (i.e. between 0 and 60 MWd/kgU), SIMULATE5 predicts volume-averaged fuel temperatures that differ between -4K to +20K with respect to the ENIGMA reference solution (see Fig. 5). Except in three cases (rods #11, #12 and #28), the maximum differences between SIMULATE5 and ENIGMA do not exceed 30K and the minimum differences are above -15K. The average of the maximum differences is 22K, and the average of the minimum differences is -1K (see Fig. 5).

### 3.2 BWR environment

Twenty-four BWR rods of different design were modelled. The cases cover most of the historical and present BWR designs (8x8, 9x9, and 10x10), the radial cold gap is between 75 microns and 110 microns, the power is between 15 kW/m and 30 kW/m; and the rod internal pressure is between 0.1 MPa and 2 MPa.

Fig. 6 compares the rise of the volume-averaged fuel temperature above the coolant temperature as a function of burnup at nominal conditions for a historical 8x8 fuel rod and a present 10x10 design. The red line represents the ENIGMA reference solution, the blue line represents the SIMULATE5 solution and the green line the differences.
Fig. 6  Fuel average temperature above coolant temperature for two typical BWR rods

Results for all BWR rods are summarized in Fig. 7 and Fig. 8. Fig. 7 shows the differences at 0 MWd/kgU (rod BOL), at 20 MWd/kgU (representative of the burnup at which the fuel-clad gap closes), and at 60 MWd/kgU (representative of an average fuel rod EOL).

Fig. 7  Averaged fuel temperature differences for all BWR rods at three different burnups

Fig. 8 summarizes for each of the twenty-four BWR rods, the maximum, average and minimum TFU differences in the burnup range 0 to 60 MWd/kgU.
From the figures above, the following observations can be made:

- At BOL (0 MWd/kgU): The agreement between the SIMULATE5 solution and the ENIGMA solution is not as good as for the PWR rods (compare Fig. 7-a and Fig. 4-a). Differences are between +10 K and +40 K. It is worth noting that the biggest differences are observed for pins belonging to older designs (Pin #2 and Pin #3).

- After one cycle of irradiation (represented by the 20 MWd/kgU data): The SIMULATE solution is in good agreement with the ENIGMA solution. The differences are within ±10 K (see Fig. 7-b).

- At EOL (represented by the 60 MWd/kgU data): The present solution differs less than 10 K with respect to the ENIGMA reference solution (see Fig. 7-c).

- In the examined burnup range (i.e. between 0 and 60 MWd/kgU), SIMULATE5 predicts volume-averaged fuel temperatures that differ between -10 K and +10 K with respect to the ENIGMA reference solution (see Fig. 8). Except in two cases (fuel rods #2 and #3), the maximum differences do not exceed 30 K, and the minimum differences are above -30 K. The average of the maximum differences is 18 K, and the average of the minimum differences is -12 K (see Fig. 8).

4. Summary

A fuel pin model for SIMULATE5 has been developed. The analysis of eighteen PWR rods and twenty-four BWR rods over the burnup range between 0 and 60 MWd/kgU allow us to conclude that the SIMULATE5 volume-averaged fuel temperatures are in good agreement with the volume-averaged fuel temperatures computed by the fuel performance code ENIGMA.

At the beginning of life, the fuel temperatures predicted by SIMULATE5 and ENIGMA are in very good agreement. As burnup progresses, the fuel temperatures predicted by SIMULATE5 follow the same trend as the ENIGMA solution. For the PWR rods, on average, SIMULATE5 predicts volume-averaged fuel temperatures that differ between -4 K to +20 K with respect to the reference solution. For BWR rods, the differences are between -10 K and +10 K.

5. References


