# MODELING OF THE COOLANT REGION IN THE ALFRED CORE

# IN CASE OF THERMAL EXPANSION

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**Abstract**

From a neutronic point of view, the effects of thermal expansion on the reactivity of a reactor core are an important feedback mechanism. It is therefore necessary to model the expanded configuration in terms of shapes, densities and volumes as accurately as possible. Unfortunately, this is not easy for those regions that expand differently due to a temperature gradient. This is the case of the coolant region along the active height, where the change in temperatures determines a change in the flow area and consequently in both the mass and volume of the coolant itself. In the study, three alternative approaches to modelling the coolant region are theoretically discussed. In the first model, masses and volumes of the expanded configuration are calculated for the entire subchannel using a single averaged pitch, and uniform density along the active height as evaluated by the average expansion of the coolant. In the second model, the first approach is enhanced by taking into account the axial change in mass, i.e., a discretization of the subchannel in regions is introduced so that in each axial region a more precise value of the coolant density can be used. Finally, in the third model, starting from the idea of explicitly preserving the reaction rates by preserving the coolant inventory compared to the real case, the mass is again calculated for each axial region in which the subchannel has been discretized but using an effective density which is derived from applying the physical density to the real-case volume of each region. These three approaches, applied to the elementary cell of the ALFRED core, are then compared by detailed analysis with MCNP6.1. This is done to assess, on one hand, their discrepancy on the reactivity of the system and, on the other hand, their demanding in terms of model setup and computational costs.

## INTRODUCTION

In a nuclear reactor core, any thermal expansion causes a variation of the geometries with consequent variation of the volumes. In materials where mass is conserved, such as solids, the new volumes cause a change in density, while in liquids or gasses both mass and density can change. To account for the effects of thermal expansion on the reactivity of the system, it is necessary to model the expanded configuration as accurately as possible. This can be done easily for those regions that are not subject to temperature gradients. By contrast, for those regions subject to a non-uniform temperature field, modelling the expanded configuration can be troublesome. This is the case of the coolant region corresponding to the active zone, where the progressive increase in temperatures determines a continuous change in the flow area: this effect is larger in fast reactors, where the temperature increase by the coolant is larger than in light water reactors. Typically, the temperatures involved here are, on one hand, those of the lower and upper support grids at the contact points with the Fuel Assembly (FA) wrapper tube (if present) which determine a different expansion of the lattice pitch as the axial height varies and, on the other hand, those of the cladding along the active region according to their typical profile. As a consequence, there are different values of the flow area from the bottom to the top of the active height, which correspond to different axial values of mass and volume, therefore of density, of the coolant.

From a neutronic point of view, the effects of the coolant density on the reactivity in steady-state but also during many postulated accident sequences depend on the reactor type. In pressurized-water reactors (PWRs), for instance, these effects concern the probability of neutrons to be moderated to thermal energies, to leak from the reactor (leakage term) and to be absorbed in the coolant (absorber term) in particular when a chemical shim, such as boron, is present. Differently, in Sodium-cooled Fast Reactors (SFRs), where the coolant slows down neutrons by inelastic scattering at high energy and by elastic scattering at low energy, these effects have to do with the neutron spectrum and with *η*, the average number of fission neutrons emitted per neutron absorbed in the fuel [1]. In the Advanced Lead-cooled Fast Reactor European Demonstrator (ALFRED) [2], the reactor taken into account in this study, these effects are again related to the neutron spectrum, and therefore to *η*, due to inelastic scattering reactions close to the MeV region. At the same time, they also concern the leakage term due to elastic scattering reactions mainly impacting between a few keV and a few MeV [3].

In order to investigate the neutronic effects due to different coolant modelling in the active region of the ALFRED core, three alternative approaches are taken into account in this study. Theoretically described at first to highlight their main differences in the calculation of volume and density, these are tested in the subchannel of the ALFRED core by detailed analyses with MCNP6.1. This comparison, by assessing, on one hand, their discrepancy on the reactivity of the system and, on the other hand, their demanding in terms of model setup and computational costs, is in fact necessary to obtain quantitative information for establishing a reference calculation route catching the aimed details while balancing the required efforts.

## CoOLANT rEgiOn MODElS

In this paragraph, the three alternative approaches to modelling the coolant region are theoretically described. For this purpose, a typical hexagonal lattice cell with height equal to the active region of the fuel pin is assumed as the reference geometry. As usual, a fuel pin made of a cylindrical cladding tube is taken into account. In the following, the subscripts *ac*, *co*, *ce* and *cl* refer respectively to the active zone, the coolant, the cell and the cladding while the superscripts 0 and *'* refer to the configurations before and after the thermal expansion. It is important to note that all differential deformations including those of the fuel pin in the active zone are assumed to stay in the linear regime.

MODEL 1

1. Calculate the average pitch (), the average outer radius of the cladding () and the active height () of the expanded configuration;
2. compute the coolant volume of the active region () as the difference between the volumes of the cell () and pin (), i.e.,

|  |  |
| --- | --- |
| ; |  |

1. determine the coolant temperature in the active region () as an average between the inlet and outlet temperatures of the active zone;
2. calculate the coolant density of the active region () corresponding to temperature ;
3. finally, compute the coolant mass of the active region () using the volume and the density .

MODEL 2

1. Calculate , and of the expanded configuration;
2. compute as the difference between and , i.e.,

|  |  |
| --- | --- |
| ; |  |

1. discretize the active region into regions of equal height with ;
2. determine, for each region, the coolant temperature () as an average between the inlet and outlet temperatures of the region;
3. calculate, for each region, the coolant density () corresponding to temperature ;
4. finally, compute the coolant mass of each region () using the volume and the density of the region.

MODEL 3

1. Discretize the active region in regions of equal height with ;
2. calculate, for each region, the average pitch ( and the average outer radius of the cladding ();
3. compute, for each region, as the difference between the expanded volumes and in the region, i.e.,

|  |  |
| --- | --- |
| ; |  |

1. calculate, for each region, the coolant temperature () as an average between the inlet and outlet temperatures of the region;
2. determine, for each region, the coolant density () corresponding to the temperature ;
3. calculate, for each region, the coolant mass () using the density and volume of the region.

These three approaches in the calculation of the volumes are shown graphically in Fig. 1 where, for each model, half of the axial section of the lattice cell is drawn distinguishing between the fuel pin in grey and the coolant region in white.



Fig. 1. Scheme of the three approaches to modelling the coolant in the active zone.

In MODEL 1, no axial changes in volume and density are taken into account, the volume and density being calculated for the entire active region. Consequently, a unique mass value for the entire active region is obtained.

In MODEL 2, the first approach is enhanced by an axial discretization of the active region in multiple regions so that a more physical description of the axial change in mass can be taken into account. At the same time, this approach does not allow to conserve, with respect to the real case, neither the total coolant mass (equal to that calculated in MODEL 1) nor its distribution along the height, the latter being overestimated in the lower part of the active zone and underestimated in the upper one. In fact, although the axial values of the coolant density are correctly calculated at the average temperature of each region, no axial change in volume is taken into account as due to the different expansions of the pitch and cladding radius along the height.

A very important aspect in the first two models has to do with choosing the average lattice pitch of the fuel pin to be used. From a geometrical point of view, it corresponds to the value in the midplane of the entire fuel pin by averaging the thermal expansions of the lower and upper support grids to which the fuel pin is radially constrained. However, this pitch, in the case of asymmetric axial position of the active region with respect to the overall pin, does not accurately represent the region of main neutronic interest. Therefore, from a neutronic point of view, the pitch computed weighting the positions of the grids with respect to the midplane of the active zone should be preferred. Analogously, the average outer radius of the cladding should be set according to the active zone rather than the entire fuel pin. To do this, the cladding should be expanded to the average temperature of the active zone.

In MODEL 3, the mass is again calculated for each axial region in which the active height has been discretized, but using specific volume and density values of that region. In fact, the MODEL 3 starts from the idea of explicitly preserving the reaction rates by preserving the coolant inventory compared to the real case. This can be done via a more accurate estimate of the volumes. Indeed, preserving the reaction rates means preserving the masses that means, in turn, preserving the volumes, the density being calculated independently as a function of temperature. This is achieved by using the pitch and radius values relative to each region and not to the whole active region as done in the first two models. Regarding the average pitch of each region (), this is calculated as the actual value of the function in the middle of each region, the function being the line passing through the points corresponding to the thermal expansions of the lower and upper support grids. Obviously, the slope of the line depends on the coolant temperature difference across the core. Regarding the outer radius of the cladding (), this is as well obtained by expanding the cladding at the actual average temperature of the region (). Ultimately, this approach solves the main drawback of the other two models, which is that the greater the distance from the midplane of the active zone, the less accurately the volumes are calculated.

It is interesting to note that in MODEL 3 a unique value of height is used in the calculation of cell and pin volumes, respectively and . By making explicit the height, the equation can be written as:

|  |  |
| --- | --- |
| . |  |

The height is obtained by axially expanding the fuel at its average temperature. Therefore, it must be

|  |  |
| --- | --- |
| . |  |

Since the cladding expands differently from the fuel, the height of the cladding that corresponds, once expanded, exactly to that of the fuel of that region can be defined as

|  |  |
| --- | --- |
| . |  |

An important aspect of MODEL 3 concerns the number of regions in which the coolant region must be discretized to minimize the modelling effects on reactivity with respect to the real case. This is, of course, a typical reactor-dependent problem to be analyzed from time to time. In the next paragraph, an assessment aimed at the ALFRED subchannel is made.

Although more accurate than the other approaches, the volumes calculated in MODEL 3 imply, however, a very complicated geometrical description due to the lack of axial continuity between the regions in which the coolant region has been discretized. To overcome this drawback, it can be advantageous to use fictitious volumes and densities instead of the real ones, the masses being preserved. To do this, a fictitious volume can be computed for each region, by using the average values of pitch and radius relative to the entire active region, respectively and , as calculated in MODELs 1 and 2. It is worth noting that the volumes thus obtained are exactly equivalent to those calculated in MODEL 2. Finally, a fictitious coolant density coherent with the real mass and the fictitious volume can be calculated.

## COOLANT MODELLING IN ALFRED

In this paragraph, the three approaches to modelling the coolant region are compared to each other on the basis of their effects on the reactivity of the ALFRED fuel assembly hexagonal lattice. To this end, two states are taken into account: the shutdown core at refuelling temperature, also called “Cold Zero-Power” (CZP) state, with all temperatures at about 380 °C, as initial state, and the core operating at full power, known as “Hot Full-Power” (HFP) state, with temperatures referring to the hottest fuel pin in the hottest FA in the lower enrichment zone, as expanded state. In the ALFRED core, the lower enrichment zone refers to the inner fuel assemblies enriched to 20.5 wt.% in PuO1.97. All geometric and material data are detailed in [4], including the correlations for the instantaneous coefficients of linear expansion as a function of temperature, , for solid materials, such as MOX (fuel), austenitic stainless steel AIM1 of class “15-15Ti” (used for all structures including cladding) and yttria-stabilized zirconia (insulator). For these materials, the total volumetric expansion is assumed to be equally distributed among the three axes, hence .

Regarding operating temperatures, the main values for fuel, cladding and coolant at HFP from which volumes and densities of the expanded configuration derive are shown in Table 1. For the two insulating pellets that protect, above and below the active zone, the metallic structures from the temperatures reached in the fuel, the temperatures are set to the inlet and outlet coolant temperatures, respectively 673.2 and 811.8 K.

Regarding lead density as a function of temperature, it is computed according to the following equation [5]

|  |  |
| --- | --- |
| , |  |

where, for temperature 𝑇 in [K], density is in [kg/m3]. This gives: 10580 kg/m3 at 673.2 K, 10567 kg/m3 at 683.2 K, 10535 kg/m3 at 708.4 K, 10495 kg/m3 at 739.1 K, 10455 kg/m3 at 770.7 K, 10419 kg/m3 at 799.1 K, 10402 kg/m3 at 811.8 K and 10494 kg/m3 at 740.1 K.

TABLE . OPERATING TEMPERATURES OF THE EXPANDED CONFIGURATION

|  |  |  |  |
| --- | --- | --- | --- |
|  | Temperature [K] | | |
| Region | MODEL 1 | MODEL 2 | MODEL 3 |
| Fuel | | | |
| Average axial temperature | 1632.6 | 1632.6 | 1632.6 |
| Cladding | | | |
| Axial temperature below active region | 673.2 | 673.2 | 673.2 |
| Average axial temperature in region 1 | - | - | 716.7 |
| Average axial temperature in region 2 | - | - | 752.3 |
| Average axial temperature in region 3 | - | - | 787.5 |
| Average axial temperature in region 4 | - | - | 816.4 |
| Average axial temperature in region 5 | - | - | 837.2 |
| Max. axial temperature | 848.9 | 848.9 | 848.9 |
| Average axial temperature | 782.0 | 782.0 | 782.0 |
| Axial temperature above active region | 811.8 | 811.8 | 811.8 |
| Coolant | | | |
| Inlet bulk temperature | 673.2 | 673.2 | 673.2 |
| Average bulk temperature in region 1 | - | 683.2 | 683.2 |
| Average bulk temperature in region 2 | - | 708.4 | 708.4 |
| Average bulk temperature in region 3 | - | 739.1 | 739.1 |
| Average bulk temperature in region 4 | - | 770.7 | 770.7 |
| Average bulk temperature in region 5 | - | 799.1 | 799.1 |
| Outlet bulk temperature | 811.8 | 811.8 | 811.8 |
| Average bulk temperature | 740.1 | - | - |

The comparison of the three models in terms of volume, mass and multiplication factor is made below. For each term, two different cases are examined related to the expanded values of pitch and cladding outer radius in MODELs 1 and 2: in case 1 (reference case) they are calculated with respect to the midplane of the active zone while in case 2 they refer to the midplane of the fuel pin between the lower and upper support grids. Unless otherwise specified, the subchannel is divided into 7 regions of which 5 in the active zone (regions 2 to 6), 1 below (region 1) and 1 above (region 7).

### Volume

The comparison between the subchannel volumes as obtained in case 1 is shown in Table 2. As expected, there are no differences between the volumes of the first and second models (column “1 vs 2”). Consequently, the relative differences between these volumes and those calculated in the third model (columns “1 vs 3” and “2 vs 3”, respectively) are the same. However, it should be noted that these differences are very small, always well below 0.1 % in the active zone.

TABLE . SUBCHANNEL VOLUMES IN CASE 1

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Subchannel region | MODEL 1  [cm3] | MODEL 2  [cm3] | MODEL 3  [cm3] | 1 vs 2  [%] | 1 vs 3  [%] | 2 vs 3  [%] |
| 1 (inlet) | 28.3280 | 28.3280 | 28.3088 | 0.000 | 0.068 | 0.068 |
| 2 | 6.1577 | 6.1577 | 6.1621 | 0.000 | -0.071 | -0.071 |
| 3 | 6.1577 | 6.1577 | 6.1591 | 0.000 | -0.023 | -0.023 |
| 4 | 6.1577 | 6.1577 | 6.1562 | 0.000 | 0.025 | 0.025 |
| 5 | 6.1577 | 6.1577 | 6.1549 | 0.000 | 0.046 | 0.046 |
| 6 | 6.1577 | 6.1577 | 6.1558 | 0.000 | 0.032 | 0.032 |
| 7 (outlet) | 7.7664 | 7.7664 | 7.7833 | 0.000 | -0.217 | -0.217 |
| Total mass (2 to 6) | 30.7885 | 30.7885 | 30.7880 | 0.000 | 0.002 | 0.002 |

To better appreciate the difference between the three approaches, the five volumes of the active zone of Table 2 are decomposed in the two volumes from which they are calculated. In fact, the subchannel volume (for the purpose of neutronic modelling) is equal to half the difference between the corresponding volumes of the cell and fuel pin. As shown in Table 3, unlike the first two models in which the volumes of the cell and fuel pin do not depend on the region, the third model calculates these volumes according to the values that the lattice pitch and cladding outer radius assume as the region varies.

TABLE . CELL AND FUEL PIN VOLUMES IN THE ACTIVE REGIONS (CASE 1)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | MODELs 1 and 2 | | MODEL 3 | |
| Subchannel regions | Cell volume  [cm3] | Pin volume  [cm3] | Cell volume  [cm3] | Pin volume  [cm3] |
| 2 | 28.8264 | 14.5110 | 26.8531 | 14.5416 |
| 3 | 28.8264 | 14.5110 | 26.8398 | 14.5300 |
| 4 | 28.8264 | 14.5110 | 26.8264 | 14.5140 |
| 5 | 28.8264 | 14.5110 | 26.8131 | 14.4948 |
| 6 | 28.8264 | 14.5110 | 26.7997 | 14.4756 |

Case 2 is reported in Table 4. In this case, the cell and pin volumes of the first two models are calculated by using 0.68551 cm instead of 0.68579 cm as half pitch and 0.52922 cm instead of 0.52964 cm as outer radius of the cladding, being the values expanded at the average axial temperature of the whole fuel pin (739.5 K). It is interesting to note that the relative difference between the total volume of the first two models and that of the third, although still modest, in case 2 is greater by a factor of 5 with respect to case 1 (0.011 % vs 0.002 %, respectively).

TABLE . SUBCHANNEL VOLUMES IN CASE 2

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Subchannel region | MODEL 1  [cm3] | MODEL 2  [cm3] | MODEL 3  [cm3] | 1 vs 2  [%] | 1 vs 3  [%] | 2 vs 3  [%] |
| 1 (inlet) | 28.3273 | 28.3273 | 28.3088 | 0.000 | 0.065 | 0.065 |
| 2 | 6.1582 | 6.1582 | 6.1621 | 0.000 | -0.062 | -0.062 |
| 3 | 6.1582 | 6.1582 | 6.1591 | 0.000 | -0.014 | -0.014 |
| 4 | 6.1582 | 6.1582 | 6.1562 | 0.000 | 0.033 | 0.033 |
| 5 | 6.1582 | 6.1582 | 6.1549 | 0.000 | 0.055 | 0.055 |
| 6 | 6.1582 | 6.1582 | 6.1558 | 0.000 | 0.041 | 0.041 |
| 7 (outlet) | 7.7124 | 7.7124 | 7.7833 | 0.000 | -0.911 | -0.911 |
| Total mass (2 to 6) | 30.7912 | 30.7912 | 30.7880 | 0.000 | 0.011 | 0.011 |

### Mass balance

As shown in Table 5 for case 1, the relative differences between the three approaches are quite small even in terms of mass. However, it should be noted that, unlike the previous term, the relative differences between the masses of the regions 2-6 of models 1 and 2 are not zero. This is due to the fact that densities calculated at different coolant temperatures are used. In fact, the average bulk temperature of the entire subchannel and those of each axial region are used, respectively, in models 1 and 2. On the contrary, the total mass obtained with the two models is equivalent, the average density of the subchannel being equal to the average of the average densities of each region.

TABLE . SUBCHANNEL MASSES IN CASE 1

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Subchannel region | MODEL 1  [g] | MODEL 2  [g] | MODEL 3  [g] | 1 vs 2  [%] | 1 vs 3  [%] | 2 vs 3  [%] |
| 1 (inlet) | 599.4030 | 599.4030 | 598.9970 | 0.000 | 0.068 | 0.068 |
| 2 | 129.2386 | 130.1346 | 130.2265 | -0.688 | -0.759 | -0.071 |
| 3 | 129.2386 | 129.7377 | 129.7679 | -0.385 | -0.408 | -0.023 |
| 4 | 129.2386 | 129.2548 | 129.2230 | -0.013 | 0.012 | 0.025 |
| 5 | 129.2386 | 128.7566 | 128.6975 | 0.374 | 0.420 | 0.046 |
| 6 | 129.2386 | 128.3093 | 128.2687 | 0.724 | 0.756 | 0.032 |
| 7 (outlet) | 161.5782 | 161.5782 | 161.9296 | 0.000 | -0.217 | -0.217 |
| Total mass (2 to 6) | 646.1929 | 646.1929 | 646.1835 | 0.000 | 0.001 | 0.001 |

No noticeable difference between Table 5 and Table 6 (case 1 vs case 2) can be observed, except for the relative difference between the total masses in the subchannel in MODELs 1 and 2 vs 3, which differ from each other by one order of magnitude (0.001 % vs 0.010 %).

TABLE . SUBCHANNEL MASSES IN CASE 2

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Subchannel region | MODEL 1  [g] | MODEL 2  [g] | MODEL 3  [g] | 1 vs 2  [%] | 1 vs 3  [%] | 2 vs 3  [%] |
| 1 (inlet) | 599.3890 | 599.3891 | 599.0226 | 0.000 | 0.061 | 0.061 |
| 2 | 129.2501 | 130.1461 | 130.2270 | -0.688 | -0.750 | -0.062 |
| 3 | 129.2501 | 129.7492 | 129.7685 | -0.385 | -0.400 | -0.015 |
| 4 | 129.2501 | 129.2662 | 129.2237 | -0.013 | -0.020 | 0.033 |
| 5 | 129.2501 | 128.7681 | 128.6983 | 0.374 | 0.429 | 0.054 |
| 6 | 129.2501 | 128.3207 | 128.2696 | 0.724 | 0.764 | 0.040 |
| 7 (outlet) | 160.4536 | 160.4536 | 160.8717 | 0.000 | -0.260 | -0.260 |
| Total mass (2 to 6) | 646.2503 | 646.2503 | 646.1872 | 0.000 | 0.010 | 0.010 |

### Multiplication factor

The criticality calculations are performed by means of the general-purpose Monte Carlo radiation-transport code MCNP6.1 [6]. A schematic view of the geometry as modeled in MCNP is given in Fig. 2.

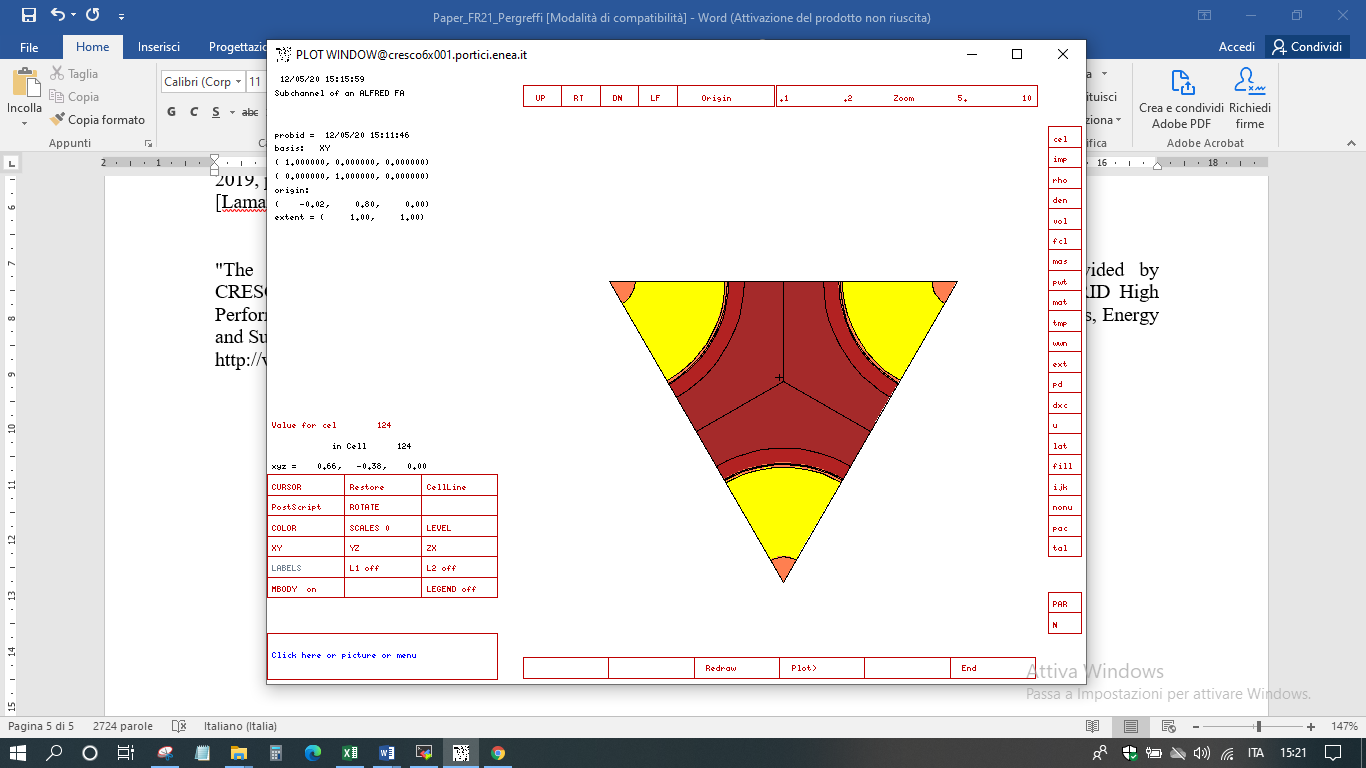


Fig. 2. Subchannel of the ALFRED cell as modelled in MCNP.

As evaluated nuclear data library, the ENDF/B-VIII.0 distribution is chosen for all calculations. According to the available set in ENDF/B-VIII.0 [7], the operating temperatures for Doppler broadening of the cross-sections are 1200 K for the fuel and 600 K and 900 K for the insulator, coolant and all structures respectively below and above the active region. Calculations are done assuming axial and radial reflective boundary conditions. To minimize statistical variations, 100 k-eigenvalue source iteration cycles, of which the first 10 skipped, with 1.0E+07 histories per cycle are used. This corresponds to a standard deviation (1σ) of the criticality values never exceeding 3 pcm. All calculations are carried out on CRESCO6, the Linux cluster composed by 434 interconnected nodes integrated in the ENEAGRID infrastructure [8]. In particular, the calculations are distributed over 60 nodes for a total of 2880 cores, increasing significantly the computational performance.

The results in terms of multiplication factor are summarized in Table 7. From their mutual comparison, it is straightforward to conclude that the effects on reactivity of the different modelling of the subchannel region corresponding to the active zone of the ALFRED FA are, in general, very small. In fact, it should be noted that the maximum discrepancy between the different models, for each case, is always within the statistical uncertainty of the calculation. A statistically significant difference emerges instead between the results of case 1 and 2 (almost the same for all models) which, in any case, is about 20 pcm. It is worth noting that in case 2 the pitch, although geometrically correct being calculated with respect to the midplane of the fuel pin between the lower and upper support grids, does not accurately represent the active zone, the region of main neutronic interest. This is due to the asymmetric axial position of the active region with respect to the overall pin, shifted upwards (and more important: in the same direction of the coolant flow) from the mid span because of the gas plenum in the bottom part, which is longer than the spring region in the top. Consequently, by assuming this pitch, the probability of fission induced by neutrons would be overestimated, the distance between the fuel pins along the active zone being indeed underestimated. Additionally – even though hindered by the assumption of reflective boundaries in the present modelling – the underestimation of the pitch would also imply an overestimation of the leakage term, which would add to the former amplifying the net effect of the pitch assumption in a real full-core calculation. In light of this, we can conclude that even if their effects on the reactivity are modest, values of pitch and cladding radius computed with respect to the midplane of the active zone should be, from a theoretical point of view, preferred.

TABLE . CRITICALITY VALUES FOR THE DIFFERENT MODELS

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| State | Subchannel model | kinf  [-] | St. dev.  [-] | kHZP – kCZP  [pcm] |
| CZP | - | 1.26281 | 0.00002 | - |
| HZP | MODEL 1 – case 1 | 1.25626 | 0.00002 | 655 |
| MODEL 1 – case 2 | 1.25652 | 0.00003 | 629 |
| MODEL 2 – case 1 | 1.25632 | 0.00002 | 649 |
| MODEL 2 – case 2 | 1.25654 | 0.00002 | 627 |
| MODEL 3 – 5 regions | 1.25631 | 0.00002 | 650 |
| MODEL 3 – 20 regions | 1.25637 | 0.00002 | 644 |

Finally, to assess the impact of the axial discretization i.e., of the number of regions in which the coolant region must be divided to minimize the modelling effects on reactivity compared to the real case, a simulation with 20 regions is performed. This means that the height of each region is reduced by a factor of 4 from 16.2 cm to 4.05 cm. As can be seen, also in this case a negligible difference can be noted, but an indication again can be retrieved. The direction of the change due to a refinement in the axial discretization of the subchannel, and the extent of the differences with the results of MODELs 1 and 2, indicate that MODEL 1 should be avoided, even though with small benefits on the accuracy of estimate, which should be judged on a case-by-case basis depending on the associated modelling effort.

Since the effects on the reactivity of the three models are modest, a key parameter in the choice of the model to be adopted becomes indeed that related to the computational costs. In this regard, it is worth distinguishing between two times: model implementation time and CPU time. Whether, in the implementation phase, the more accurate physical description of MODEL 3 – 5 regions takes longer than those of MODELs 1 and 2, an opposite trend can be observed in terms of CPU time. In fact, a time saving of 2.5% and 5% should be noted going respectively from MODEL 1 – case 1 to MODEL 2 – case 1 and from MODEL 2 – case 1 to MODEL 3 – 5 regions. This trend is not confirmed if we include the MODEL 3 – 20 regions. In fact, the latter model, which requires the longest implementation time, takes substantially the same CPU time as MODEL 1 – case 1, i.e., 7% more time than that of MODEL 3 – 5 regions.

## CONCLUSIONS

Three alternative approaches to modelling the coolant region along the active height have been compared relatively to the non-uniform temperature field which determines a continuous change in the flow area and consequently in both the mass and volume of the coolant itself. These models have been first generalized to better describe their main differences in the calculation of volume and density, then tested in the subchannel of the ALFRED cell by detailed analyses with MCNP6.1 to investigate their effects on reactivity, to be compared with the associated modelling and computational efforts.

From a theoretical point of view, the main difference between the models has to do with the fact that MODEL 3 allows to explicitly preserve the reaction rates by preserving the coolant inventory compared to the real case through a more accurate estimate of the volumes and therefore of the masses, the density being calculated independently as a function of temperature. It should be noted that mass here means both the total coolant mass and its distribution along the active height. Conversely, both MODELs 1 and 2, even though to different degrees of refinement, stand on the assumption of considering the subchannel geometry (as due to the lattice pitch and the rod diameter) uniform along its axial development.

In the case of the subchannel region corresponding to the active zone of the ALFRED FA, two types of effect on reactivity are observed: that due to the choice of the reference expanded values of pitch and cladding outer radius, and that due to the modelling approach per se. In both cases, the observed differences are very small; however, some considerations can be drawn. Concerning the first effect, discrepancies are statistically appreciable, being about 20 pcm, between choosing the expanded values of the pitch and cladding outer radius with respect to the midplane of the active zone or to the midplane of the whole fuel pin (i.e., between the lower and upper support grids). In this case, a clearer indication can be drawn in favour of referencing the expanded values of the pin diameter and lattice pitch to the midplane of the active region for the sake of reactivity evaluation. This conclusion is further enforced considering the potential additional effect that can be anticipated in extending the test simulations presented to the whole ALFRED core. In fact, since the average distance between the fuel pins is overestimated, the core diameter would be overestimated, as would, in turn, the leakage term, with a negative bias on the reactivity of the system.

Relatively to the modelling approach, although the one-to-one difference (at most 6 pcm) is not statistically appreciable, a trend can be observed with respect to the simulation performed with a more refined axial discretization of the subchannel, which indicates the tendency of MODEL 1 to underestimate reactivity. Moreover, if we add the fact that the implementation of MODEL 3 takes longer than that of MODEL 2 (and 1), it can be concluded that MODEL 2 could represent an appropriate trade-off between the correctness of the simulation and the affordability of the modelling effort.

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