A PROPOSED PARAMETERIZATION OF INTERFACE DISCONTINUITY FACTORS DEPENDING ON NEIGHBORHOOD FOR PIN-BY-PIN DIFFUSION COMPUTATIONS FOR LWR

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ABSTRACT

There exists an interest in performing full core pin-by-pin computations for present nuclear reactors. In such type of problems the use of a transport approximation like the diffusion equation requires the introduction of correction parameters.
Interface discontinuity factors can improve the diffusion solution to nearly reproduce a transport solution. Nevertheless, calculating accurate pin-by-pin IDF requires the knowledge of the heterogeneous neutron flux distribution, which depends on the boundary conditions of the pin-cell as well as the local variables along the nuclear reactor operation. As a consequence, it is impractical to compute them for each possible configuration.
An alternative to generate accurate pin-by-pin interface discontinuity factors is to calculate reference values using zero-net-current boundary conditions and to synthesize afterwards their dependencies on the main neighborhood variables. In such way the factors can be accurately computed during fine-mesh diffusion calculations by correcting the reference values as a function of the actual environment of the pin-cell in the core.
In this paper we propose a parameterization of the pin-by-pin interface discontinuity factors allowing the implementation of a cross sections library able to treat the neighborhood effect. First results are presented for typical PWR configurations.

Key Words: interface discontinuity factor, pin-by-pin computations, neighborhood effect.

1. INTRODUCTION

Full core pin-by-pin diffusion or SP3 solutions are achievable for three dimensional and multigroup full core calculations in a reasonable amount of time, while direct solutions of the transport equation are still too demanding for a production code in such type of problems, more over if thermal-hydraulics coupling and time evolution are considered.

However, the use of the diffusion approximation needs the introduction of correction factors to nearly reproduce the solution that would be obtained with a transport method. The Generalized Equivalence Theory (GET) [1] and the Superhomogenization method (SPH) [2] are the most extended approaches. Besides, it is also possible to define different interface discontinuity factors (IDFs) than those of GET based on a black-box behavior or Selengut normalization [3].

In any case those factors should be calculated for the entire heterogeneous system if seeking to exactly reproduce the transport solution. Since in practice those accurate factors will not be

available, only a few transport calculations of the pin cells in infinite lattice or embedded in some configurations representative of the fuel assemblies are computed, in order to generate all the parameters used during the full core diffusion calculation.

Considering that the boundary conditions of any pin-cell in the true core environment differ from the zero-net-current condition normally used in the heterogeneous transport calculations, then the computed correction factors will differ from those generated in the infinite lattice case.

An alternative to generate accurate factors is to calculate reference values using zero-net-current boundary conditions and to find a suitable representation of these factors depending on the position of the pin inside the fuel assembly when the boundary conditions differ from zero-net-current. In such way, the IDF could be treated as any other cross section during the parameterization of the library, but including some specific parameters representing the differences in the pin-cell neighborhood from the cases considered in the generation of the library.

This paper suggests a possible parameterization of the IDFs to treat the neighborhood effect based on observation of the behavior of their values in different configurations and on the Analytic Coarse-Mesh Finite Difference (ACMFD) expressions for the diffusion equation [4] which have been further tested by our group for nodal core calculations [5].

The adjustment of the coefficients can be made by running a small number of neighborhood cases compared to the high number of possible configurations to be encountered in a full core, thus reducing the amount of computational time needed to treat this effect if all the possible cases were to be considered.

Preliminary results computed with the diffusion pin-by-pin code COBAYA3 [6] show a positive implementation of such factors for two different configurations of 5x5 pins clusters, different from the 3x3 clusters used to parameterize the IDFs for typical PWR configurations.

2. PARAMETERIZED INTERFACE DISCONTINUITY FACTORS

2.1. Definitions of the correction factors

Three possible correction factors have been considered for the present study, the ones from the SPH method, the classical GET interface discontinuity factors and the Selengut interface discontinuity factors.

SPH factors are defined so as to preserve both the reaction rates and the streaming of neutrons from one pin or node to its neighbors. To that aim a multiplicative factor μ is introduced in the cross sections, which has to be obtained by an iterative procedure using the lower order formulation in the homogenized system and using expressions in (1).

$$\tilde{\Sigma} \cdot \bar{\phi}^{hom} = \Sigma \cdot \bar{\phi}^{het}$$
$$\tilde{\Sigma} = \mu \cdot \Sigma$$
$$\mu = \frac{\bar{\phi}^{het}}{\bar{\phi}^{hom}} \tag{1}$$

The factors generated with the SPH method are not direction dependent, but cell dependent and some parameterizations have already been investigated [7, 8]. They are not suitable for our purposes as the mixing of the effect of all the cell interfaces in just one parameter will make the search of the neighborhood dependencies tougher.

GET interface discontinuity factors f_G are defined as the ratio of the heterogeneous interface flux ϕ_s^{het}, the one coming from the transport solution; and the homogeneous interface flux ϕ_s^{hom}, the one obtained from the expressions used in the diffusion solver (2). They are defined so as to preserve the interface flux and net current at the interfaces from the transport solution by correcting the finite difference expression for the interface current as in equation (3) where h is the cell width.

$$f_G = \frac{\phi_s^{het}}{\phi_s^{hom}} \tag{2}$$

$$J^{het} = -D \cdot \frac{\phi_s^{het} / f - \bar{\phi}^{het}}{h/2} \tag{3}$$

As these factors are interface dependent, they contain information representing the orientation and position of the cell inside its environment. For instance, they are able to reflect the effect of a rotation of the environment around the cell, while SPH method is not able to separate that effect for each interface. So they will facilitate our search of a parameterization depending on neighborhood.

In the particular case of a pin in infinite lattice the homogeneous interface flux is equal to the homogeneous average flux, which by definition will coincide with the heterogeneous one if the reaction rates are to be preserved; therefore we obtain a simpler expression for the GET factor f_0 equal in all the interfaces (4).

$$J^{het} = 0 \Rightarrow \phi_s^{hom} = \bar{\phi}^{het} \Rightarrow f_0 = \frac{\phi_s^{het}}{\bar{\phi}^{het}} \tag{4}$$

For the case where the pin is not in an infinite lattice, the discontinuity factors are different for each interface as the currents are, and they cannot be computed without obtaining the homogeneous interface flux corresponding to our lower order solution (5), e.g. diffusion.

$$\phi_s^{hom} = -\frac{J^{het} \cdot h}{2 \cdot D} + \bar{\phi}^{het} \tag{5}$$

Selengut interface discontinuity factors f_S are defined so as to preserve the partial currents at the interfaces $J_{\pm}^{het}$ from the transport to the diffusion solution (6). They enter inside the diffusion equation in the same way as the GET factors (3), so no further developments are needed inside the diffusion solver to use them. They are different from the GET interface discontinuity factors since the GET definition only preserves the partial currents if the higher order operator used to obtain the heterogeneous fluxes is also diffusion, while Selengut factors preserve these partial currents for any higher order operator [3].

$$f_S = 2 \cdot \frac{J_{-}^{het} + J_{+}^{het}}{\phi_s^{hom}} \tag{6}$$

In our case, GET and Selengut interface discontinuity factors were computed and used to study the goodness of the parameterization.

2.2. Configurations considered to generate the interface discontinuity factors

To perform the study, 4 types of fuel pins, 1 guide tube pin and 1 control rod pin were used, all with a common cell pitch of 1.26 cm. The gap between fuel and cladding was not modeled.

The four types of fuel pins are a UOX 4.2 $^{w}/_{0}$, the same UOX pin containing Gadolinium, a MOX pin with 5.2 $^{w}/_{0}$ enrichment in Plutonium and another MOX pin with 7.8 $^{w}/_{0}$ enrichment. The control rod is a Silver, Indium and Cadmium (AIC) alloy.

Specifications for each pin and the two 5x5 clusters considered to test the parameterization were taken from a NURESIM [9] benchmarking document [10]. And all the transport computations were performed with the NEWT code from the SCALE6.0 code package [11] and its ENDF/B-5 library in 44 energy groups suitable for light water reactors.

A small subroutine was created to post-process the NEWT output file and get all the quantities in a more manageable format, including the computation of both GET and Selengut IDFs. The capability of using a NEWT output file as a cross section library file for COBAYA3 was also implemented, so the reference calculation could be reproduced by COBAYA3 with the generated interface discontinuity factors.

First, all the fuel pins were computed with reflective boundary conditions with a critical buckling search. Cross sections and interface values, including partial and net currents and fluxes, were obtained from NEWT in 5 different energy group structures featuring 1, 2, 4, 8 and 11 energy groups from the initial 44 energy groups calculations, for comparison purposes. The interface values were used to generate the single cell interface discontinuity factors as defined in equations (2) and (6).

Afterwards, different sets of 3x3 pin clusters with reflective boundary conditions were defined in order to perturb the partial currents at the interfaces of the fuel pin from the zero-net-current condition, being able to study the dependency on neighborhood of the computed IDFs for these interface (cross sections changes due to neighborhood were neglected).

The configurations are formed by the same fuel pin used in the infinite lattice case fulfilling the entire cluster except for the central position where a different type of pin was defined as sketched in Figure 1.

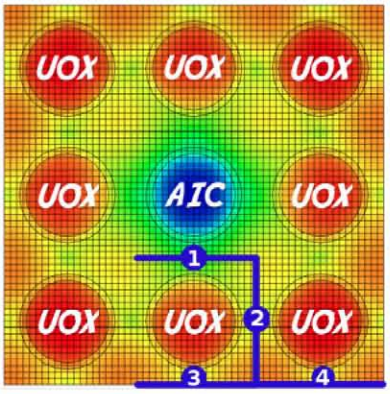

Figure 1. Arrangement for the 3x3 clusters and interfaces of interest

The UOX pin was perturbed with a water hole, a Gadolinium pin and a control rod; the Gadolinium pin was perturbed with a water hole, a UOX pin without Gadolinium and a control rod. On the other hand, the MOX fuel pins have been only perturbed with a water hole and a control rod, as Gadolinium is not present in such assemblies; uranium pins could have also been used to perturb the MOX clusters.

From the results obtained for each perturbation, only the 4 interfaces numbered in Figure 1 yield new information about the interface discontinuity factors due to the symmetries. Note that interface number 2 produces information for two cells to its left (2L) and right (2R).

2.3. Comparison of the different interface discontinuity factors

The interface discontinuity factors computed from the cases defined above have been represented against different values considered to be important as neighborhood parameters. Let's first pay attention to the dependence of the IDFs with energy by representing their value for each energy group.

Figure 2 shows the values of the GET factor for the single UOX fuel pin, this value is equal for all interfaces. From the 44 energy groups' representation it is clear that most of the correction is needed in the thermal range.

The representations for 4 and 8 energy groups are in good agreement with the 44 groups profile above the thermal range while some lost of information in the thermal range is noted. The profiles of the IDF for the Selengut definition are quite similar to the ones of GET but with slightly different values.

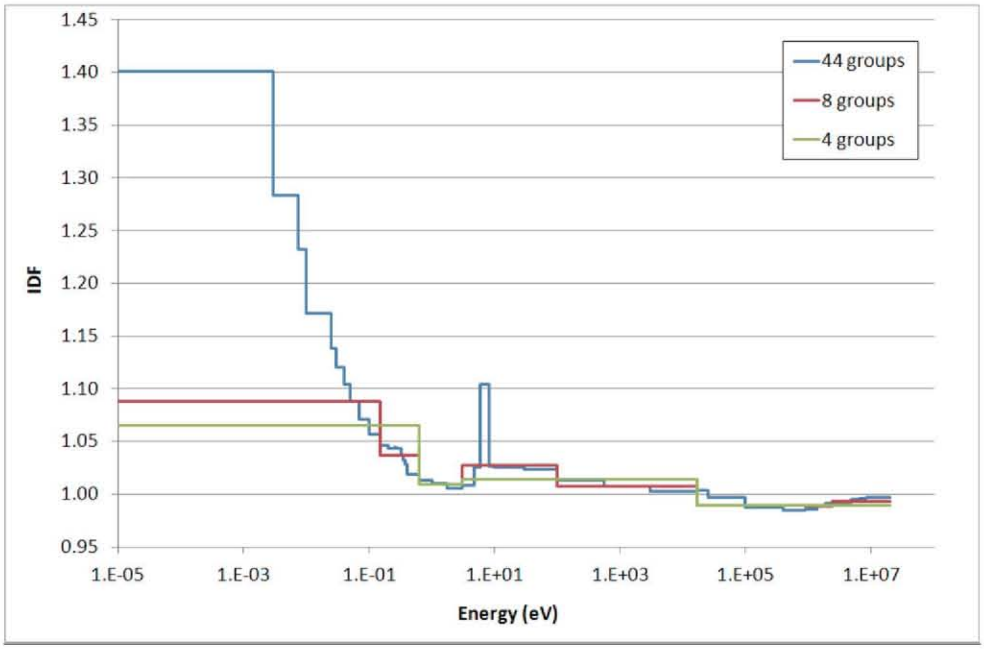

Figure 2. GET interface discontinuity factors for the UOX single cell

The IDFs for the 3x3 cluster represented in Figure 1, where the UOX fuel pin boundaries are perturbed with a control rod in the central position, were computed. Figure 3 shows the difference between those computed IDFs and the single cell values in 4 energy groups.

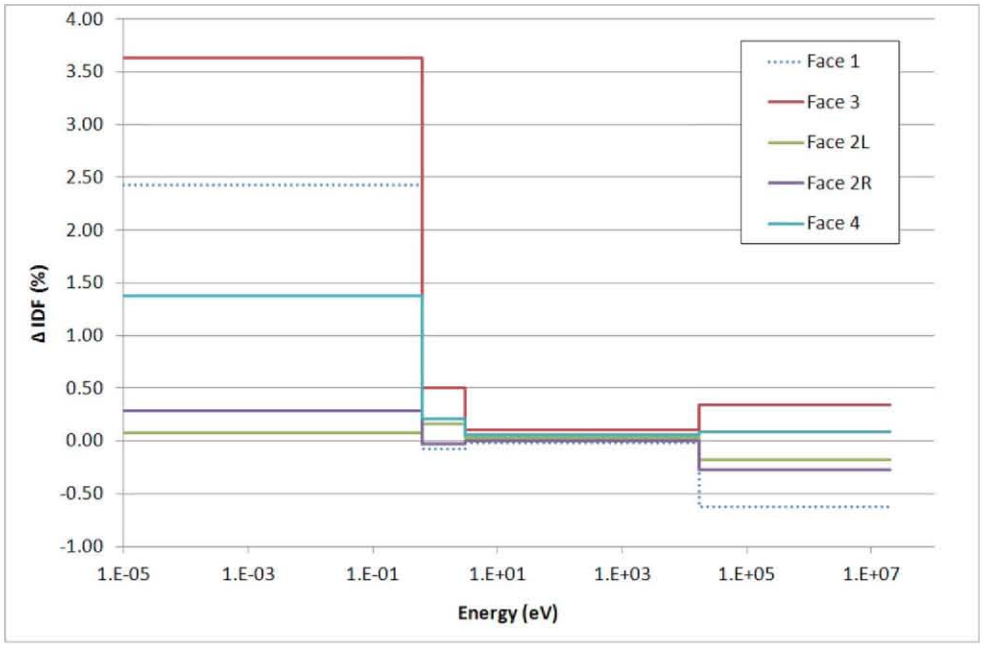

Figure 3. IDF differences between a perturbed case and the single cell calculation

This gives an idea of the correction level to be introduced by our parameterization which is always lower than 10% for the cases considered, which indicates that the non linear iteration to compute the parameterized IDF should converge to levels below 10% to result in an improvement of the calculations.

2.4. Proposed parameterization of the interface discontinuity factors

The ACMFD formulation for homogeneous nodes comes out explicitly from the analytic solution of the multigroup diffusion equations, with no approximation in 1D problems [4].

It relies on the transformation of the physical space of group fluxes into the modal space of the complete base of eigenvectors of the multigroup diffusion equation matrix. The resulting ACMFD coupling equations (7) are matrix-vector relations and, in this sense, it can be considered as a higher-order scheme with respect to the FMFD diffusion approximation, since it includes the effects of the intra-cell flux shape and the spectral variation.

$$\left|\phi\right\rangle_{(\pm h/2)} = A^{f}\cdot\left|\bar{\phi}\right\rangle \mp \frac{h}{2}A^{j}\cdot D_{g}^{-1}\cdot\left|J\right\rangle_{(\pm h/2)} - R^{-1}\left|T_{m}\right\rangle_{(\pm h/2)} \tag{7}$$

In this equation, the quantities represented as $\left|kets\right\rangle$ are vectorial ones containing the value of the flux or the current for all the energy groups, A^{f} and A^{j} are matrices affecting the vector fluxes and currents respectively coming from the analytical solution of each mode, R matrices come from the diagonalization of the diffusion system matrix and change the base from the physical to the modal space; $\left|T_{m}\right\rangle$ is the transverse leakage term – arising from the generalization of the 1D ACMFD expression to more dimensions – expressed in the modal space; and h is the cell width.

If we consider the GET definition of the IDF and introduce the ACMFD expression to obtain a higher-order approximation of the interface flux, we get relation (8). In this equation, divisions are made component by component. D stands for the diffusion coefficient, λ_{m} is the eigenvalue associated to the solution of mode m, and L^{het} is the transverse leakage in the physical space coming from the transport solution.

$$\left|f_{G}\right\rangle = \frac{\left|\phi^{het}\right\rangle_{(\pm h/2)}}{\left|\phi^{hom}\right\rangle_{(\pm h/2)}} = \frac{A^{f}\cdot\left|\bar{\phi}^{het}\right\rangle \mp \frac{h}{2}A^{j}\cdot D_{g}^{-1}\cdot\left|J^{het}\right\rangle_{(\pm h/2)} - \left(I - A^{f}\right)D_{g}^{-1}\lambda_{m}^{-1}\left|L^{het}\right\rangle_{(\pm h/2)}}{\left|\phi^{hom}\right\rangle_{(\pm h/2)}} \tag{8}$$

Here, we can identify the first summand as the IDF that would be obtained from the infinite lattice case f_{0} . While the rest of terms give an idea of what quantities would be suitable to take as neighborhood parameters, namely *the heterogeneous interface current divided by the homogeneous interface flux* and *the heterogeneous transverse leakage divided by the homogeneous interface flux*.

In practice, the previous expression seems to be not enough to catch the effect and also the cell buckling $\left|B^{2}\right\rangle$ has to be included. In principle considering the effect of the buckling from all the

energy groups over each other, and this is why we preserve also a matrix formulation represented by matrix terms $[M]$.

And as the IDF here is computed as a perturbation of the one coming from the infinite lattice calculation, we use as a third parameter *the difference between the buckling of the heterogeneous case and the buckling of the infinite lattice case* $\left|B_o^2\right\rangle$ as shown in equation (9).

$$\left|f_G\right\rangle = \frac{\left|\phi^{het}\right\rangle_{(\pm h/2)}}{\left|\phi^{hom}\right\rangle_{(\pm h/2)}} = \left|f_0\right\rangle \mp \left[M^J\right] \cdot \frac{\left|J^{het}\right\rangle_{(\pm h/2)}}{\left|\phi^{hom}\right\rangle_{(\pm h/2)}} - \left[M^L\right] \cdot \frac{\left|L^{het}\right\rangle_{(\pm h/2)}}{\left|\phi^{hom}\right\rangle_{(\pm h/2)}} + \left[M^B\right] \cdot \left(\left|B^2\right\rangle - \left|B_0^2\right\rangle\right) \qquad (9)$$

To keep the parameterization simple we neglected the dependence of each group on the rest of groups, thus changing the matrix coefficients to scalars and greatly simplifying the interpolation process, because we just need three coefficients m^J, m^L and m^B for each energy group to be adjusted using equation (10).

$$f_g = \frac{\phi_g^{het}}{\phi_g^{hom}} = f_{0g} + m_g^J \cdot \frac{J_g^{het}}{\phi_g^{hom}} + m_g^L \cdot \frac{L_g^{het}}{\phi_g^{hom}} + m_g^B \cdot \left(B_g^2 - B_{0g}^{\ 2}\right) \qquad (10)$$

This same type of parameterization has also been tested for the Selengut IDF, although the derivation was made from the GET definition of the interface discontinuity factor.

One last comment has to be added for the pins without fuel material, for which it is not possible to compute infinite lattice solutions without an external source. In these cases the parameterization is performed leaving the f_0 factor as a variable offset yielded by the interpolation process instead of being fixed from the single cell computations and using only the buckling as the parameter without a reference value.

3. COMPUTATION AND APPLICATION OF THE PARAMETERIZATION

3.1. Results from the least squares interpolation

All the gathered data have been arranged in a single file including all the energy groups, interfaces and types of clusters considered. The code R for statistics [12] has been used to treat these data and study the dependencies of the IDFs on interface values and buckling.

In particular, the IDFs have been represented against the parameters already described in the previous section to test for linearity on the dependencies. Prospection was made for different numbers of energy groups and for both definitions of the IDF, GET and Selengut.

Reasonably good agreement was encountered for all the energy groups considering the amount of simplifications done to get equation (10). Following, there are examples of the IDF's behavior against the parameters.

Next figures show the IDF values for a UOX fuel pin when changing its neighborhood according to Figure 1. The represented values correspond to the thermal group in a 4 group-energy structure.

In Figure 4, the IDF is represented versus the variation of the current to homogeneous interface flux. Trend lines are included for each interface numbered in Figure 1, showing a linear dependence.

The reason to use one trend line per interface number is that the mixture of effects is different for each interface, and also because of the difference in the cell buckling depending on the pin considered.

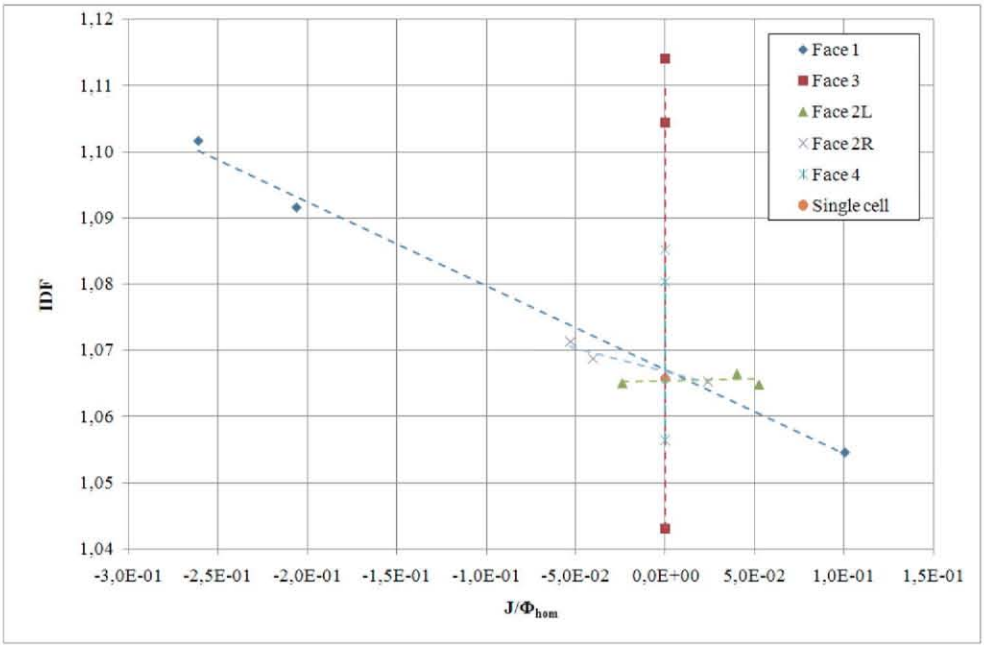

Figure 4. Dependence of GET IDF vs. interface current to homogeneous interface flux

Figure 5 shows the linear dependence of the IDF against transverse leakage to homogeneous interface flux and Figure 6 against the difference between the cell buckling and the single-cell buckling value.

Figure 5 shows a good linear fitting while the dependence with the cell buckling is more scattered. The inclusion of the buckling didn't come from the ACMFD equations but from observation of the results and it is a good choice as represented in Figure 6. The cell buckling represents all the effects which are not included in the other two parameters, as the true expression which should be used for the heterogeneous flux is not the ACMFD expression for diffusion, but the one for transport [13] that has additional terms.

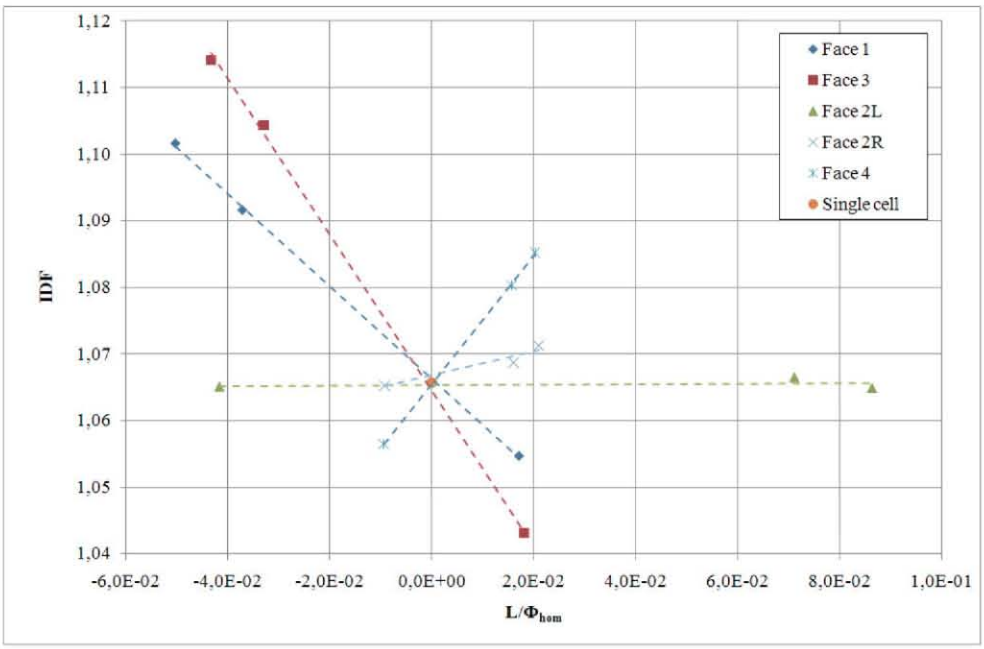

Figure 5. Dependence of GET IDF vs. transverse leakage to homogeneous interface flux

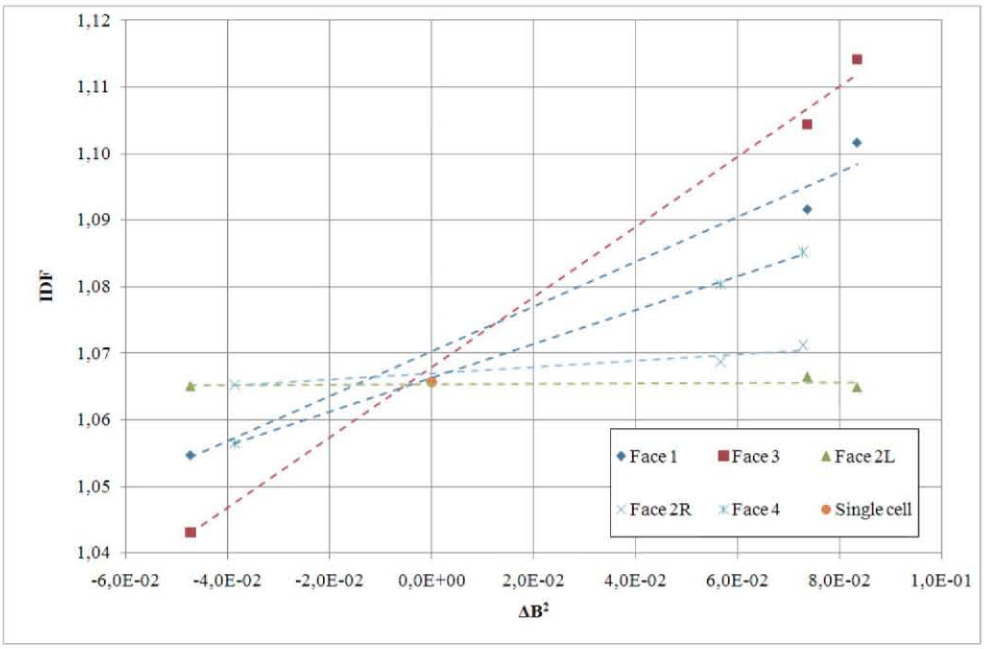

Figure 6. Dependence of GET IDF vs. the buckling change from the single cell case

The comparison between the adjustment of the GET definition and the Selengut one presented a better fitting for the later. Moreover, the use of the parameterized Selengut coefficient inside COBAYA3 showed to be more stable than the use of the GET coefficient.

3.2. Testing of the parameterization with 5x5 clusters

Two 5x5 clusters were used to test the parameterization: A is representative of a MOX fuel assembly including two water holes, three medium Pu enrichment fuel pins, and rest of higher enrichment Pu fuel pins; and B is representative of a UOX fuel assembly including two water holes and one Gadolinium pin.

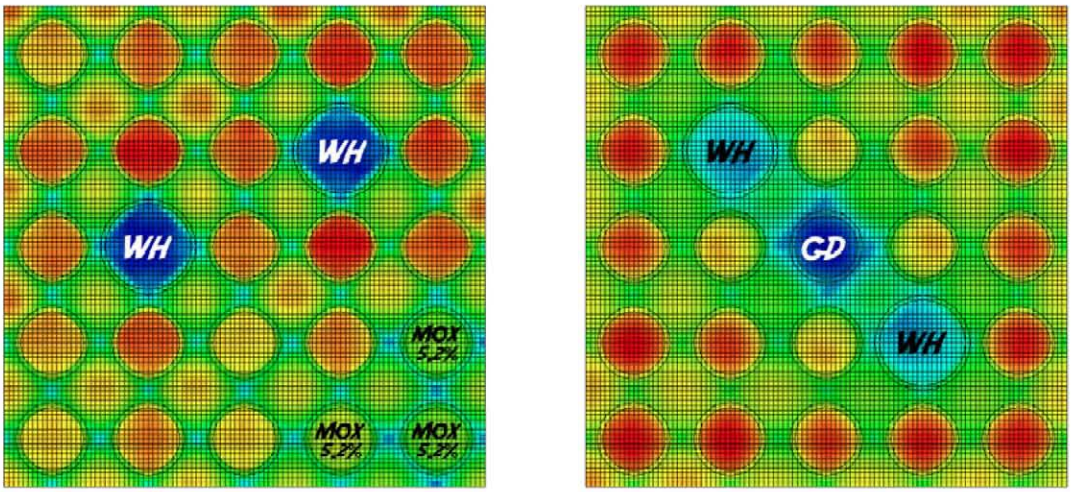

Figure 7. 5x5 pins clusters defined to test the parameterization A and B

Both clusters have been solved with NEWT and reference values for the homogenized and collapsed cross sections and for the IDF per interface were produced. The use of such values in the pin-by-pin diffusion solver COBAYA3 reproduced the results of the NEWT calculation in k effective and pin power distribution, as expected.

In order to test the goodness of the parameterized IDF the same calculation was repeated with COBAYA3, first without using any IDF, then using the IDF produced by the single cell computations which are equal on each interface of the pin, and then using the parameterized discontinuity factors.

The results in k effective and the maximum relative pin power error are presented in Table I and Table II for the two configurations considered. Although results without any IDF correction seem to be good, this is not true in general, and more challenging problems are being defined but results are not available at the moment.

Table I. Comparison of results with reference for cluster A (MOX pins)

	Reactivity difference (pcm)	Maximum pin power factor relative difference (%)
No IDF correction	-117	0.97
Single cell IDF	-115	1.01
Parameterized IDF	-50	0.69

Table II. Comparison of results with reference for cluster B (UOX pins)

	Reactivity difference (pcm)	Maximum pin power factor relative difference (%)
No IDF correction	67	0.47
Single cell IDF	1014	1.41
Parameterized IDF	-36	0.47

In any case, Table II is a clear example of the bad performance of the single cell IDF at the pin-by-pin level, similar to the use of the ADF at the assembly level for nodal codes but where this type of factor work quite well, the error here goes from 1014 pcm to -36 pcm in k-eigenvalue. When considering interface dependent discontinuity factors the results are improved in both cases with very good results.

Even more important than the low differences with respect to the transport solution is the fact that the IDF non-linear iteration converged to levels below 5 % in relative error difference, enough to consider them converged.

In order to achieve convergence of the IDF iteration, which is performed outside the k-eigenvalue loop, a damping on the calculated IDFs had to be used as high as 0.95 to avoid instabilities of the iteration. With this damping value the number of recomputations of the IDF starting from the single cell value was of 116 for cluster A and 100 for cluster B for the mentioned 5% level of convergence. However, next iterations start from a distribution very close to the new solution so the computational time is much lower.

4. CONCLUSIONS

An original expression to parameterize the interface discontinuity factors used for diffusion computations has been presented. Two different definitions for the interface discontinuity factor have been considered, GET and Selengut, with the second one resulting in a more stable choice when parameterized.

The proposed parameterization comes from the use of ACMFD expressions for the diffusion equation, and it has been further simplified neglecting the cross terms between energy groups; and further expanded by including the cell buckling to compensate effects not included in the ACMFD expression, giving a simple relationship suitable to be used in pin-by-pin diffusion codes.

The interpolation coefficients have been derived using transport results from NEWT and applying a least squares adjustment with the statistical code R. The resulting values have been tested on small clusters using the COBAYA3 pin-by-pin diffusion code with a positive evaluation.

Further testing must be performed using problems involving a higher number of pins, like fuel assembly clusters, and with stronger heterogeneities, for instance introducing UOX and MOX

elements, burnup, control rods configurations and configurations representative of the core boundary with baffle and reflector elements. These problems will intensively test the convergence capability of the interpolation process which has a non-linear aspect that needs to be more deeply studied.

In summary, the generated expressions are able to catch the neighborhood effect in a very simple and practical way and are a good base for further developments in such kind of parameterization.

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