CASL-U-2015-0258-000

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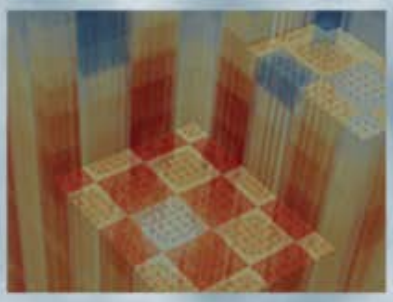

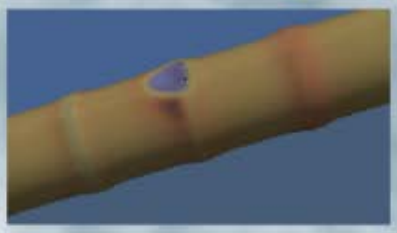

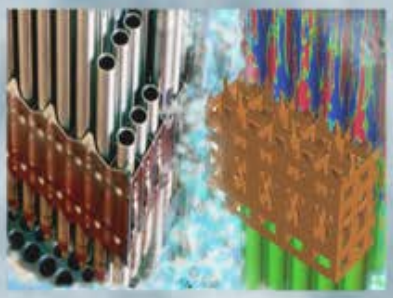

**Jipu Wang, Bill Martin**
*University of Michigan*

**Benjamin Collins**
*Oak Ridge National Laboratory*


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# Sensitivity Study of MOC Parameters with VERA Benchmark Cases

Jipu Wang[1] (jipuwang@umich.edu), Benjamin Collins[1,2] (collinsbs@ornl.gov), Bill Martin[1] (wrm@umich.edu)
[1]Department of Nuclear Engineering and Radiological Sciences
University of Michigan, Ann Arbor, MI 48109
[2]Oak Ridge National Laboratory, Oak Ridge, TN 37831

## MOTIVATION

- Method of Characteristics (MOC) has become the workhorse for solving neutron transport equation, in which $k_{eff}$ is an essential part of the solution.

$$\vec{\Omega}\cdot\nabla\varphi(\vec{r},\vec{\Omega},E)+\Sigma_t(\vec{r},E)\varphi(\vec{r},\vec{\Omega},E)=\frac{\chi(\vec{r},E)}{4\pi k_{eff}}\int_0^{\infty}\nu\Sigma_f(\vec{r},E)\int_0^{4\pi}\varphi(\vec{r},\vec{\Omega}',E')d\Omega'dE'+\int_0^{\infty}\int_0^{4\pi}\Sigma_s(\vec{r},\vec{\Omega}'\cdot\vec{\Omega},E'\to E)\varphi(\vec{r},\vec{\Omega}',E')d\Omega'dE'$$

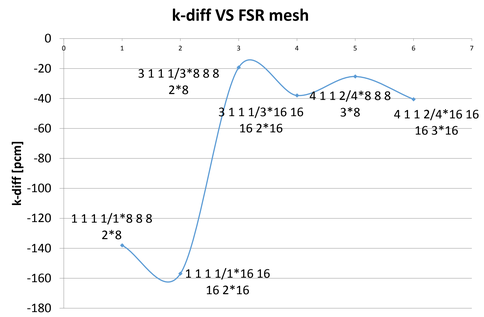
- However, the sensitivities of MOC solution to its parameters are not well known. This study is aimed at evaluating the sensitivities of k-diff to MOC parameters for selected VERA benchmark cases, where k-diff is the difference between keff for the specific cases and keff for the most highly resolved case.
- The solution responses to varying parameters are investigated and this helps i) identify the importance of each parameter and ii) generate suggested range of parameters that can give adequate accuracy and still keep relatively low computational cost.
- This study will also impart important insights to the application of Method of Manufactured Solutions (MMS) in the solution verification process.

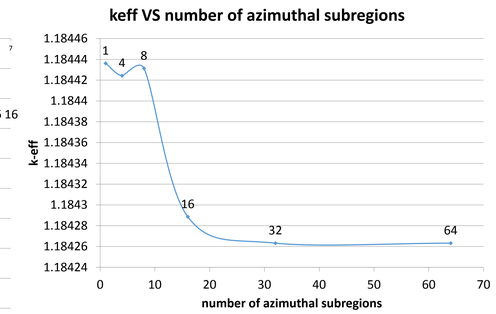
## METHODOLOGY

- **Benchmark Cases**
  The selected VERA benchmark cases cover small pincell problems (1a, 1e) as well as relatively larger assembly problems (2a, 2l) as well as problems involving very small regions such as an IFBA coating (1e, 2l).
- **Input Parameter Space**
  The input space of MOC parameters includes
  - Flat Source Region (FSR) mesh
    - Radial discretization: 1 1 1 1, 3 1 1 1, 4 1 1 2. (listings of number of radial subdivisions in fuel, gap, cladding and moderator)
    - Azimuthal discretization: 8, 16
  - Quadrature Set Order
    - Azimuthal angle, Chebyshev: 8, 12, 16, 20, 24, 28, 32
    - Polar angle, Yamamoto: 3
  - Ray Spacing [cm]
    - Non-IFBA case (1a, 2a): 0.08, 0.05, 0.02, 0.01, 0.005
    - IFBA case (1e, 2l): 0.08, 0.05, 0.03, 0.01, 0.008, 0.005, 0.003, 0.002, 0.001, 0.0008, 0.0005, 0.0003, 0.0002, 0.0001.
- **Other specifications**
  - MPACT Version: v1.0.0
  - Cross Section Library: mpact47g_e70r0_TCP0.xsl
- **Data acquisition and post-processing**
  - A python script runs each case with all parameter combinations in the input space after which keff is gathered and summarized for post processing.
  - keff's from all cases are sorted and grouped in sequence by each dimension of the multidimensional parameter space to reveal keff sensitivity to each of the MOC parameters.
  - Extra cases are run for further investigation of some oscillating features of keff to ray spacing and Chebyshev quadrature set order.
  - Extra azimuthal discretization cases are used to reflect azimuthal symmetry in determining adequately fine ray spacing.

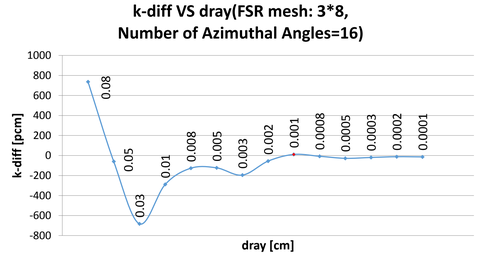
## RESULTS

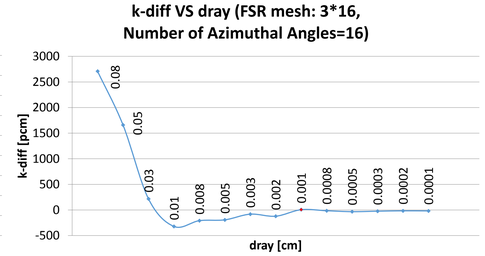
- **Sensitivity to FSR mesh (e.g. VERA 1a)**



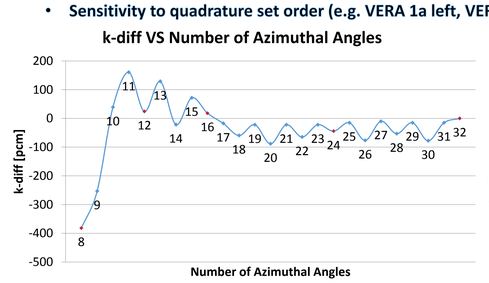



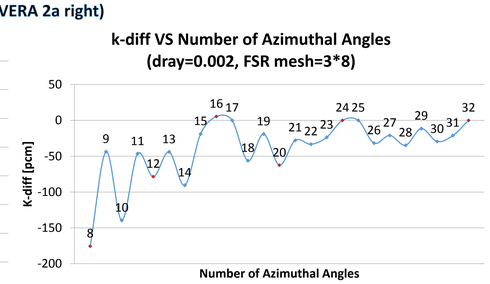

- **Sensitivity to ray spacing (e.g. VERA 1e)**




- **Sensitivity to quadrature set order (e.g. VERA 1a left, VERA 2a right)**




## OBSERVATIONS

| MOC Parameter | Sensitivity | Observations (VERA 1a) |
|---|---|---|
| FSR mesh | Slight | Adequate accuracy is obtained as long as the FSR mesh is not too coarse - 3 rings in fuel and 2 rings in moderator for radial discretization and 8 slices for azimuthal discretization are suggested. |
| Angular quadrature | Moderate | k-diff changes drastically when quadrature set order is changed - 16 azimuthal angles in (0, PI/2) and 3 polar angles in (0, PI/2) are suggested. |
| Ray spacing | High | k-diff oscillates with dray, but after dray decreases to 0.01 cm, the amplitude of oscillation is bounded within ±50 pcm range, so 0.01 cm is suggested. |

| MOC Parameter | Sensitivity | Observations (VERA 2a) |
|---|---|---|
| FSR mesh | Slight | k-diff is only slightly sensitive to FSR mesh, adequate accuracy is obtained as long as the FSR mesh is not too coarse - 3 rings in fuel and 2 rings in moderator for radial discretization and 8 slices for azimuthal are suggested. |
| Angular quadrature | Moderate | k-diff is still sensitive to the quadrature set order, although to a smaller extent. Order 16 and 3 is suggested, after which the amplitude of oscillation is bounded and going to higher order up to 32 only gives at most another 50 pcm accuracy. |
| Ray spacing | High | k-diff is much less sensitive to ray spacing – the maximum accuracy gained by reducing dray from 0.08 to 0.005 cm is only 35.2 pcm in this input space, average accuracy gain being 16.8 pcm. So for a problem that does not involve very thin regions, ray spacing as large as 0.08 cm or even larger is quite acceptable if k is the only concern. Note it is possible that the local pin power resolution still requires smaller ray spacing.<br>The dray dependency of the k-diff vs Number of Azimuthal Angles curve pattern is less profound since k-diff is less sensitive to dray. |

| MOC Parameter | Sensitivity | Observations (VERA 1e) |
|---|---|---|
| FSR mesh | Slight | k-diff is only slightly sensitive to FSR mesh as long as the ray spacing is decreased to a value that is comparable to the IFBA coating thickness (0.001 cm). Moreover, in order to have the right dependency behavior – k-diff barely depends on azimuthal discretization - a ray spacing at least as small as 0.002 cm (twice the coating thickness) should be used. Otherwise, k-diff drastically depends on the number of azimuthal zones used, which is unphysical in an "azimuthally symmetric" case. Again, 3 rings in fuel and 2 rings in moderator for radial discretization and 8 slices for azimuthal discretization are suggested. |
| Angular quadrature | Moderate | k-diff is sensitive to quadrature set order. It changes profoundly when quadrature set order changes, similar to vera_1a. However, it is not easy to find an order after which the oscillation will be bounded within a small range when the ray spacing is not small enough, which indicates a greater sensitivity to quadrature set order in IFBA pin case. 28 azimuthal angles have to be used to bound k-diff within ±50 pcm range. Roughly, 16 azimuthal angles and 3 polar angles are acceptable. |
| Ray spacing | High | k-diff is very sensitive to ray spacing – i) when dray is too large, it causes an abnormal dependency on FSR azimuthal mesh as mentioned earlier; ii) only after the dray decreases to the coating thickness (0.001 cm) should the k-diff fall into an acceptable range, although the k-diff VS dray curve levels off earlier in some cases. |

| MOC Parameter | Sensitivity | Observations (VERA 2l) |
|---|---|---|
| FSR mesh | Slight | k-diff is only slightly sensitive to FSR mesh, adequate accuracy is obtained as long as the FSR mesh is not too coarse – 3 rings in fuel and 2 rings in moderator for radial discretization and 8 slices for azimuthal discretization are suggested. However, this is only true when the ray spacing is below 0.01 cm – ten times the thickness of the IFBA coating. This threshold value used to be 0.001 cm in Problem 1e, indicating lower sensitivity of k-diff to dray in larger problems. |
| Angular quadrature | Moderate | k-diff is still sensitive to the quadrature set order, although to a smaller extent. Order 16 and 3 is suggested, after which the amplitude of oscillation is bounded and going to higher order gives only another 10 pcm accuracy. This value used to be 50 pcm in Problem 1e, indicating mitigated sensitivity to angular quadrature in this larger problem. |
| Ray spacing | High | k-diff is less sensitive to ray spacing – the average accuracy gained by reducing dray from 0.005 to 0.0001 cm is only 50 pcm in this input space, the average accuracy gain being 24 pcm when dray is reduced from 0.003 to 0.0001 cm. So when k is the only concern, a dray as large as 0.005 cm would be OK, which is relaxed 5 times from the value 0.001 cm required by a single IFBA pin in Problem 1e.<br>The dray dependency of the k-diff vs Number of Azimuthal Angles curve pattern is barely seen, which is due to the mitigated sensitivity to Number of Azimuthal Angles and dray. |

## CONCLUDING REMARKS

1. For all cases, the sensitivity of keff to the FSR mesh is low as long as the FSR mesh is not too coarse and the ray spacing resolves the smallest region (i.e., the IFBA coating). The conclusion is that 3 rings in fuel and 2 rings in moderator for radial discretization and 8 slices for azimuthal discretization are sufficient, given a sufficiently fine ray spacing.
2. For all cases, the sensitivity of the results to the quadrature set is moderate and a reasonable set is 16 azimuthal angles per quadrant and 3 polar angles per hemisphere. In problems involving very thin region, a higher quadrature set order may be needed.
3. The sensitivity of keff to the ray spacing is strong and the ray spacing needs to be comparable to the thickness of the smallest region, such as an IFBA coating, in order to get adequate accuracy.
4. There are nonlinear relationships among the MOC parameters and their impact on keff and this makes it difficult to determine an optimum set of MOC parameters that will hold for all cases, especially when taking into account computational time. For example, the FSR mesh is not a continuously changing variable and keff oscillates with the ray spacing and the number of azimuthal angles, which means that the change in keff due to a change in either of these quantities is a function of the other variable.
5. If there were better corrections for the IFBA region (or any other thin regions of interest, say the peripheral fuel region) that could considerably reduce the sensitivity of keff to the ray spacing and angular quadrature set, then a coarser ray spacing and possibly less azimuthal angles can be used to reduce the computational cost while still retaining adequate accuracy.
6. Overall, sensitivities of keff to the FSR mesh, angular quadrature, and ray spacing are mitigated in problems with a larger computational domain. However, large problems involving very thin regions shows stronger sensitivity to MOC parameters than those without very thin regions.

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