A Simplified Model and MATLAB Code for Modelling Mo-99-Producing CANDU Bundles in the Context of an Undergraduate Nuclear Engineering Design Course

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Abstract

Undergraduate-level nuclear engineering design courses focus, among other things, on elements of fuel bundle design. Real-life CANDU fuel-bundle design involves performing accurate neutronic and thermal-hydraulic calculations by using neutron-transport codes, sub-channel-level hydraulic codes and solving the heat-conduction equation explicitly in each fuel pin. Allowing undergraduate students to simply use such codes as black boxes is unsatisfactory from a pedagogical perspective, while involving students in the development of such codes is usually beyond the scope of an undergraduate course. At the same time, the problem is complicated enough as not to be amenable to a purely analytical solution. Under these conditions, a fruitful approach is to use simplified models which undergraduate students can use to develop simple numerical computational tools. This work presents the development of a simplified model and MATLAB code which calculates the infinite multiplication factor, pin power distribution, fuel centerline temperature and Mo-99 yield for a CANDU-type bundle for different fuel pin radii, pitch circle radii and fuel enrichment. The model uses a Wigner-Seitz equivalence between a square lattice cell and a circular one. The latter is subsequently analyzed using one-group one-dimensional diffusion in cylindrical geometry. The diffusion equation is discretized using finite differences. The inverse-power iteration method is used to calculate the infinite multiplication constant and flux. The resulting flux is used to calculate the power, fuel temperature and Mo-99 production in each fuel ring.

1. Introduction

Mo-99 is an important radionuclide for clinical diagnostic applications, as it is used to produce Tc-99m. Mo-99 is produced primarily in research reactors as a fission product of U-235. The NRU reactor in Chalk River produces approximately half of the world's supply of Mo-99, but it is scheduled to cease production in 2016. One possible production alternative is to use specially-designed Mo-99-producing bundles in CANDU reactors [1, 2]. The design of such bundles involves altering some of the parameters of the regular CANDU bundle (e.g. enrichment, fuel-pin diameter, etc.), with implications on the power distribution between different fuel rings, fuel temperature and Mo-99 production in each fuel ring. Designing such a Mo-99-producing bundle constitute an interesting case study for an undergraduate nuclear engineering design course. In the preliminary design phase, it is customary to investigate a relatively large number of bundle configurations and the implications of different design options. For such preliminary design activities, as well as for teaching purposes, it is useful to have a tool able to predict the quantities of interest with minimal

computational effort, even at moderate accuracy. This report details the development of a simple MATLAB computational tool for assessing the infinite lattice multiplication constant, the Mo-99 production rate, the pin power distribution and fuel centreline temperature in a Mo-99-producing CANDU-type fuel bundle. The variable input parameters are the fuel pin radii, the pitch circle radii ring-by-ring fuel enrichment, total bundle power and coolant temperature.

2. Geometrical Model

A Wigner-Seitz equivalence is used to transform the square lattice cell into an annular cell of the same total area. The annular cell is divided into five concentric homogeneous annular regions, one for each fuel ring (including central pin) and one for moderator. The four regions corresponding to fuel rings are assumed to contain a homogeneous mixture of fuel, clad and heavy water. The moderator region contains a mixture of heavy water and calandria and pressure tube material. As a first approximation, each region's neutronic macroscopic cross sections are calculated based on its material composition using simple volume-weighted homogenization (Ring-specific pin radius and fuel enrichment are allowed.). For more advanced applications, the cross sections can be found using a lattice-level transport calculation followed by flux-weighted homogenization and group condensation.

3. Computational Approach

3.1 Mo-99 Yield

In order to determine the molybdenum yield, a set of two differential equations needed to be solved; the equation for U-235 burnup in the reactor, and the equation for the rate of change of Mo-99 within the fuel. The uranium burnup equation is:

(1)

And the Mo-99 concentration equation is:

(2)

By solving these two equations, a formula can be found for the concentration of Mo-99 in the fuel with respect to time:

(3)

While time is an important factor in this equation, the neutron flux can also vary. Because of this, the fuel's position in the reactor and power rating must both be considered. The following graph shows how the Mo-99 yield of a standard CANDU fuel bundle varies according to time and neutron

power:

Figure 1: Mo-99 Concentration at Selected Power Levels

It can be observed from this graph that the peak production occurs at around 18 days, independent of power or fuel enrichment. However, the Mo-99 yield in each ring depends on the flux/power level in that particular ring.

3.2 Infinite Multiplication Constant, Flux Profile and Pin Powers

The neutron flux in each annular region is determined using one-group diffusion theory. The diffusion equation is expressed in polar coordinates and discretised using finite differences. The general form of the diffusion equation is, with customary notations:

(4)

In the above equation, is the Laplacian of the neutron flux, is k_{eff}, and ,, , and are the number of neutrons released per fission, diffusion coefficient, macroscopic absorption cross section, and macroscopic fission cross sections respectively. Equation (4) is expressed in polar coordinates for the case with azimuthal symmetry as:

(5)

The first derivative of the flux can be approximated using finite differences:

(6)

In eq. (6), h, denotes the size of radial meshes. The annular cell can be split into an arbitrary number of equal-thickness radial meshes. The second derivative in eq. (5) is also approximated using finite differences:

(7)

(8)

By letting , , and , eq. (5) the finite-difference approximation of eq. (5) can be rewritten in as follows:

(9)

(10)

Equation (10) represents a linear eigenvalue-eigenvector problem in the form Before continuing, boundary conditions must be defined.

For this one dimensional cylindrical problem, there is a symmetry condition at the center (zero derivative) and a reflective boundary condition (zero derivative) at the edge of the moderator. These conditions imulate an infinite lattice. By applying the reflective boundary condition at the center, (n=1) one finds The linear equation incorporating this boundary condition is given by:

(11)

By applying the reflective boundary condition at the edge of the lattice (n=N), it is found that . The linear equation incorporating this boundary condition is given by:

(12)

The set of linear equations which represent an infinite lattice in cylindrical coordinates is now complete. The flux profile and k_{eff} are found through inverse power iterations.

From the finite differences approximation it was found that the system of linear equations is of the form . Subscript *m* is be used to denote the iteration number, a single underline will represent a vector, and a double underline will represent a matrix. The algorithm for inverse power iterations begins with an initial guess (*m*=1) for the flux profile A vector full of ones is sufficient. The initial value of k-eff can also be taken to be equal to one. The flux at iteration *m+1* is solved based on the flux at iteration *m* by solving:

(13)

By letting and , k-eff is calculated as follows:

(14)

The iterative process continues until the maximum absolute difference in the normalized flux profile is less than a specified tolerance (ie). The resulting flux profile is illustrated in Fig. 2.

Figure 2: Radial Flux Profile

The vertical lines in the above graph denote the separation between the four homogenized fuel ring regions and the moderator region.

The fission rate density and pin power in each fuel ring are reconstructed by dividing the total fission rate (power) in the respective radial region by the volume of the fuel in that region.

3.3 Fuel Centerline Temperature

With the pin powers available, it now becomes possible to calculate the fuel centreline temperature. The first key step in determining the centerline temperature of the fuel is to find the linear power rating of the fuel by multiplying the volumetric heat generation rate by the cross-section area of the fuel pin

With the linear power density of a pin now in hand, the centerline temperature is solved for using a thermal resistance network [3]:

(14)

4. Conclusions

The developed tool allows for the rapid evaluation of bundle configurations which would be impossible to determine based on analytical expressions thus significantly aiding the bundle design process. The model's strengths include speed and ease of use. The MATLAB code gives a quick approximate solution based on enrichment within a few seconds. Combined with the ability to easily change enrichment and other parameters in a short time, this code allows for multiple bundle designs to be tested relatively quickly. Another benefit of using MATLAB is that any part of the code can be changed or adapted; including the constants/equations used or even what is output or plotted. The main shortcoming is accuracy. Even if the tool has modest accuracy, favourable configurations can be identified and later analysed with more accurate codes (e.g. DRAGON). It should be noted that while the tool is not as accurate as a transport code, the actual results trend in the same manner as more accurate programs. As the run time for each configuration is very short (seconds), multiple changes can be made to each configuration to evaluate effects that changes in one parameter can have on another. The program is an effective teaching tool, as students can very easily see the effects each change has on the overall model performance.

5. References

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