MULTIDIMENSIONAL REACTOR KINETICS MODELING* 

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Introduction 

There is general agreement that for many light water reactor transient calculations, it is necessary to use a multidimensional neutron kinetics model coupled to a thermal-hydraulics model in order to obtain satisfactory results. These calculations are needed for a variety of applications for licensing safety analysis, probabilistic risk assessment (PRA), operational support, and training. The latter three applications have always required best-estimate models, but in the past applications for licensing could be satisfied with relatively simple, but conservative, models. By using more sophisticated best-estimate models, the consequences of these calculations are better understood, and the potential for gaining relief from restrictive operating limits increases. Hence, for all of the aforementioned applications, it is important to have the ability to do best-estimate calculations with multidimensional neutron kinetics models coupled to sophisticated thermal-hydraulic models.

This need coincides with the fact that in recent years there has been considerable research and development in this field with modelers taking advantage of the increase in computing power that has become available. This progress has now led to coupling multidimensional neutron kinetics models to the nuclear steam supply system (NSSS) thermal-hydraulics. This is not new as modelers for training simulators have always had such a coupling. What is new is that the coupling can now be done with very sophisticated models, and the planning of this coupling and the requisite modeling can take advantage of the experience of many code developers in many countries. Indeed, the point of this paper is to present one view of the current situation and to recommend what might be done in the future.

Specifically, this paper reviews the status of multidimensional neutron kinetics modeling which would be used in conjunction with thermal-hydraulic models to do core dynamics calculations, either coupled to a complete NSSS representation or in isolation. In addition, the paper makes recommendations as to what should be the state-of-the-art for the next ten years. The review is an update to a previous review of the status as of ten years ago. The general requirements for a core dynamics code and the modeling available for such a code, discussed in that review, are still applicable. The emphasis in the current review is on the neutron kinetics assuming that the necessary thermal-hydraulic capability exists. In addition to discussing the basic neutron kinetics, discussion is given of related modeling (other than thermal-hydraulics). The capabilities and limitations of current computer codes are presented to understand the state-of-the-art and to help clarify the future direction of model

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aThis paper is meant to be applicable to boiling water reactors (BWRs) and to pressurized water reactors of both Western design (PWRs) and Russian design (VVERs).
development in this area. This is to answer the question as to whether existing capabilities are sufficient or whether additional development work is needed.

The paper is organized as follows. First, the basic multidimensional neutron kinetics model is discussed. This is the heart of a core dynamics capability, but ancillary models also need to be discussed. These are treated in a following section. Next is found a section discussing the specific applications of these codes. In addition to demonstrating the need for multidimensional neutron kinetics, this section also shows how the applications determine other modeling that should be present. In the last section, comments are given on state-of-the-art codes and how these might be a first step in fulfilling future needs.

The Basic Multidimensional Neutron Kinetics Model

The basic multidimensional neutron kinetics model that is currently the state-of-the-art and is expected to be applicable to LWR applications for the expected future is based on the 3-dimensional neutron diffusion equation for two neutron-energy groups and with six groups of delayed neutron precursors. Several solution methods are considered state-of-the-art although those that are expected to be most applicable in the future utilize a nodal method to handle the spatial dependence and direct integration to handle the temporal dependence. In the following, we first consider the basic equations and then consider the solution methods.

For LWRs, a 2-group diffusion theory approach has proven to be adequate for steady-state applications, and, for those transient applications where direct validation is possible, it also has been found to be adequate. One could argue that more energy groups or a higher order approximation to the angular dependence of the neutron flux (i.e., a more rigorous approximation to the transport equation than diffusion theory) might improve the rigor of the methodology. However, since there is an interest in making the transient analysis compatible with steady-state core calculations, and since there is no direct evidence that these higher order methods give more accurate results, 2-group diffusion theory should continue to be the standard approach.\(^6\)

Six delayed neutron precursor groups are the standard for treating LWRs, and no change should be made in this area either. However, it should be noted that these properties should be defined for each computational cell throughout the core. Although this is the practice in some state-of-the-art codes, some transient codes currently in use use global averages for the delayed neutron parameters.

The equations are to be solved in three dimensions using rectangular or hexagonal geometry. Multidimensional kinetics should be equated with 3-dimensional kinetics for the simple reason that there is no need to consider 1-dimensional or 2-dimensional models. The latter two approximations are only applicable for certain transients when there is separability between the axial and radial changes during a transient. Furthermore, both of these approximations require considerable analysis in order to obtain nuclear data that have been properly averaged over the remaining dimensions (e.g., over the radial plane when the axial direction is explicitly modeled). This complicates the analysis and negates any simplification that might result from using a lower order spatial representation. Hence, it has become well-established that only 3-dimensional methods are of interest.

Note that this does not preclude the use of point kinetics models when the neutronic response of the core is not of primary importance. A code which models the NSSS should have the ability to use point kinetics with parameters supplied by the user or calculated from the 3-dimensional neutronics model—an approach not conducive to automation. One aspect of the point model that is easy to relate to the multidimensional core model

\(^6\)NESTLE (see discussion of current code capability below) uses up to four energy groups and could be used to assess the effect of the number of groups.

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is the decay heat model which can utilize the calculated steady-state power distribution to obtain decay heat loads throughout the core.

The basic equations for neutron kinetics (3-dimensional diffusion theory in two groups) can be solved in many different ways. An excellent recent review of these methods exists\(^2\), and, hence, they will not be discussed herein in any detail. It is sometimes convenient to separate the solution methods for the space dependence from those for the time dependence. For the space dependence, it is either nodal methods or coarse-mesh diffusion theory (CMDT) methods that are the most successful in terms of accuracy per unit of computation. Within these categories, it is perhaps transverse-integrated nodal methods that are the best. “These methods produce results that are comparable to those of fine-mesh finite difference calculations at a small fraction of the computational cost. The success of these methods is due to their ability to use large computational mesh boxes ... without sacrificing accuracy or limiting the type of information that may be obtained. The use of coarse computational mesh in space ... results in a dramatic decrease in the number of unknowns—and hence computer resources—while the high order spatial treatment within a node, coupled with the use of advanced homogenization procedures, maintains the accuracy at the level of the more expensive fine-mesh calculations. Dehomogenization methods have been developed which allow the determination of detailed intranodal flux and power distributions despite the coarseness of the mesh used for the nodal solution.”\(^2\)

Implicit in the use of nodal (or course-mesh) methods is that fuel assembly properties can be appropriately homogenized in order to use the large mesh of a nodal model. This is generally the case in spite of the fact that the homogenization is usually done by calculating an isolated assembly, i.e., without regard to the correct boundary conditions. However, with the introduction of discontinuity factors, it is possible to enhance the accuracy. These factors are defined for each assembly (along with the cross sections) in order to account for some of the heterogeneity in the assembly. Dehomogenization is also important because accuracy on a fuel-rod basis requires using a flux reconstruction algorithm.

The spatial solution method requires boundary conditions which are frequently at the boundary of the fueled region. At this boundary, complicated geometries and materials make it difficult to get accurate results. It is important that the boundary conditions (either at the edge of the fueled region or elsewhere) be sufficiently rigorous so that the accuracy of the method does not degrade at the boundary.

The time dependence can be treated with a direct or indirect approach. The best example of the latter is the improved quasistatic method (IQS). The IQS is based on a space-time factorization so that the spatial dependence can be solved using time steps much larger than used for the global power. Although this allows for flexibility in choosing time steps, the time steps are eventually determined by the rate at which the spatial shape is changing. Direct methods are indeed more direct and can be used in conjunction with time-step algorithms which improve the computational efficiency of the process. These algorithms allow for time steps to vary according to a set of criteria and may even allow for backstepping (the repeating of a calculational step) if necessary. In the same way that nodal methods have improved the efficiency of solving the spatial problem, new algorithms for solving sparse matrices have improved the efficiency of solving for the time dependence so that direct methods are most appropriate to use. Because of the stiffness of the neutron kinetics equations, implicit integration methods are used to advance the time.

**Other Modeling Important to a Reactor Kinetics Capability**

The neutron kinetics model is the heart of a core dynamics computer code, but there are many other components to consider when putting together a complete package. The thermal-hydraulics model is the most obvious but is not the subject of this paper. The additional models that are discussed below are how to initialize the problem, the cross section model, and the power generation model.
It must be recognized that in order to do transient calculations, it is necessary to first have a steady state. The static form of the neutron kinetics equations is an eigenvalue problem, and the eigenvalue is equivalent to the multiplication factor for the steady-state core. A problem can be initialized in various ways. The parameters that determine the initial statepoint of the reactor are the power level, the control rod pattern, the boron concentration (for PWRs and VVERs), and inlet temperature, subcooling and flowrate. If these are all consistent, then one should obtain an eigenvalue of unity indicating that the reactor is just critical (steady state) at this statepoint. In practice, the eigenvalue is close to, but not equal to, unity. It is important that the code be able to search for either the power level, control bank position, boron concentration, or inlet condition to reach a particular eigenvalue (ideally unity) to represent a proper statepoint. This capability should be built into the steady state part of the calculation.

Another type of steady state that could be of interest is a fixed-source problem where the reactor is at shutdown conditions with an external (i.e., non-fission) source enabling the multiplication. A code with this steady-state capability would allow for much wider flexibility in treating different initial conditions for transient problems.

In setting up initial conditions, it is necessary to include the effects of xenon and samarium. The distribution of these nuclides throughout the core can be calculated using the formulae for their equilibrium concentrations. However, it is a relatively straightforward addition to also include the appropriate fission product chains so that these distributions can be obtained for different slowly changing conditions (i.e., "xenon transients") in order to have additional flexibility in starting transients from different initial conditions.

Cross sections must depend on all the thermal-hydraulic feedback and control variables, i.e., fuel temperature, coolant temperature and density, boron concentration, and the presence of control rods. The fuel temperature can be an effective temperature based on the temperatures calculated by the fuel rod heat conduction model, e.g., a function of pellet average and centerline temperatures. For BWRs, an effective coolant density and boron concentration can also be defined to account for voiding and boron in the bypass channel. This is connected to a need to have the bypass region represented in more detail than just as a single channel. The dependence of the cross sections on the above variables can be specified either through analytic functions (typically polynomials) or through a sophisticated table look-up. The cross section functions/tables must be specified for each mesh box along with the delayed neutron parameters and discontinuity factors for that mesh box. The spatial dependence of the cross section functions is due to changes in fuel assembly design and burnup throughout the core. Burnup dependence is usually through up to two independent variables, exposure (GWd/ft), and some other parameter that expresses the history of the bundle germane to spectral effects. Exposure weighted void or coolant density history are the most common of these parameters.

Implicit in the discussion of the cross section representation is the need for a methodology to calculate these quantities. Although the methodology is beyond the scope of this paper, it is necessary to emphasize that the neutron kinetics capability can only be used if this methodology exists.

The power generation model takes the fission rate, adds decay heat, and distributes the heat generation rate in fuel and coolant regions. The decay heat contribution may become important when starting a transient from low power or after shutdown of the fission power. Decay heat functions can be specified according to exposure throughout the core and used in conjunction with a steady-state power distribution when the neutron kinetics is not needed.

Applications of 3-Dimensional Neutron Kinetics

The specific types of transient calculations that require multidimensional neutron kinetics when analyzing PWRs and VVERs are listed in Table 1. These applications influence the modeling that should be present in a computer code beyond the basic multidimensional neutron kinetics. Although the emphasis in this paper is on reactor
physics modeling, some applications also point to the need for special thermal-hydraulics modeling. For example, the first two transients in the list are calculated as part of a plant’s safety analysis. In order to accurately represent the cooling of the core, it is important to know the inlet temperature distribution across the core. This may be available from a 3-dimensional, thermal-hydraulic model for the vessel or from some other special mixing model.

The third item in the list, the rod ejection accident, is the design-basis reactivity-initiated accident. The consequences of this accident as well as of most other accidents need to be evaluated in terms of fuel rod response rather than bundle-average response. This means that if a calculation is done with planar meshes that are the size of fuel assemblies (or even quarters of assemblies), modeling must be present to do the dehomogenization or flux reconstruction in order to obtain fuel rod response. This also implies that a multichannel thermal-hydraulic model may be necessary in order to properly calculate the DNBR (departure-from-nucleate-boiling ratio).

The fourth item, boron dilution events, refers to any scenario that might be possible during shutdown, ascent to power, or full power operation. This requires the accurate modeling of boron transport through the system as well as the ability to represent a distribution across the core inlet as was necessary for the cold water transients discussed above.

Transients without scram refer not only to the most limiting event, which is likely caused by a loss of feedwater at beginning of cycle, but also to a spectrum of events that might be important to analyze as part of a PRA. The last event in the table refers to the fact that for operational support (e.g., for determining setpoints) or training, it may be necessary to calculate transients in which it is important to note the response of incore and excore instrumentation. This requires that these instruments be modeled and that their connection to the reactor protection system and any control system also be modeled.

Table 1: PWR Transients for which Multidimensional Neutron Kinetics is Important

<table>
<thead>
<tr>
<th>PWR Applications</th>
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<tbody>
<tr>
<td>Steam line break</td>
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<tr>
<td>Startup of cold loop</td>
</tr>
<tr>
<td>Rod ejection accident</td>
</tr>
<tr>
<td>Boron dilution events</td>
</tr>
<tr>
<td>Transients without scram</td>
</tr>
<tr>
<td>Instrumentation response</td>
</tr>
</tbody>
</table>

Table 2 shows the list of events for BWRs for which multidimensional neutron kinetics modeling is needed. Again, a review of these events sheds light on the ancillary modeling that is needed. Overpressurization events and inlet disturbances of both temperature and flowrate are analyzed as part of the licensing safety analysis. Some of the inlet perturbations (e.g., due to trip of one recirculation pump) should be specified as a function of position across the inlet, and this requires either 3-dimensional modeling in the vessel or some multichannel model which will supply the appropriate core boundary conditions. These events along with the rod drop accident require knowing conditions in individual fuel rods, and, hence, dehomogenization or flux reconstruction is needed when using codes that use meshes the size of bundles.

Transients without scram highlight the need for a boron transport model that will model flow in individual channels including bypass channels.

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Table 2  BWR Transients for which Multidimensional Neutron Kinetics is Important

<table>
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<tr>
<th>BWR Applications</th>
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<tbody>
<tr>
<td>Overpressurization events</td>
</tr>
<tr>
<td>Core inlet temperature disturbances</td>
</tr>
<tr>
<td>Core inlet flow disturbances</td>
</tr>
<tr>
<td>Rod drop accident</td>
</tr>
<tr>
<td>Transients without scram</td>
</tr>
<tr>
<td>Stability analysis</td>
</tr>
<tr>
<td>Instrumentation response</td>
</tr>
</tbody>
</table>

Current Computer Codes

It is instructive to look at the state-of-the-art in order to understand how much modeling capability that could be used for an advanced reactor analysis package already exists and how much might have to be developed. The focus here will be on codes in the U.S. although some of these codes are also used abroad.

One example of a code that is in the public domain that has many of the desirable features discussed above is NESTLE\(^3\). The code uses the NEM approach and is applicable to both rectangular and hexagonal geometry. It does steady-state searches to solve the eigenvalue problem and has many other features that are desireable but peripheral to the discussion herein. Examples of these are the option of using four neutron energy groups, of using a finite difference method rather than the NEM, and the ability to calculate the adjoint (steady-state) problem (useful in deriving point kinetics parameters). NESTLE has been integrated into system thermal-hydraulic codes (TRAC and RELAP5\(^4\)).

There are several other similar codes that are in use in proprietary or special circumstances. There are also several codes that are currently in use which may not be considered state-of-the-art, but, nevertheless, they are used successfully for a range of applications and a study of their characteristics is informative and necessary for designing a new capability. These other codes are listed in Table 3 along with some special notes that identify unique features.
### Three-Dimensional Core Kinetics Codes Currently in Use

<table>
<thead>
<tr>
<th>Code</th>
<th>Special Modeling Features</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>NESTLE&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Two-group NEM</td>
<td>Coupled to system thermal-hydraulic codes</td>
</tr>
<tr>
<td>SIMULATE-3K&lt;sup&gt;5&lt;/sup&gt;</td>
<td>Two-group NEM or semi-analytic nodal method</td>
<td>Has excore system models</td>
</tr>
<tr>
<td>ARROTTA&lt;sup&gt;6&lt;/sup&gt;</td>
<td>Two-group ANM</td>
<td>Coupled to RETRAN for LWR analysis</td>
</tr>
<tr>
<td>NEM/TRAC&lt;sup&gt;7&lt;/sup&gt;</td>
<td>Two-group NEM</td>
<td>Coupled to TRAC-PF1 for PWR applications</td>
</tr>
<tr>
<td>SPNOVA&lt;sup&gt;8&lt;/sup&gt;</td>
<td>Two-group nodal method with approximation (G-matrix method)</td>
<td>For PWR applications</td>
</tr>
<tr>
<td>RAMONA&lt;sup&gt;9&lt;/sup&gt;</td>
<td>1½ energy groups, CMDT</td>
<td>Used for BWR applications</td>
</tr>
<tr>
<td>TRACG&lt;sup&gt;10&lt;/sup&gt;</td>
<td>One group, CMDT, IQS</td>
<td>Coupled to the TRAC code for BWR applications</td>
</tr>
<tr>
<td>DIF3D-K&lt;sup&gt;11&lt;/sup&gt;</td>
<td>Multigroup, direct or IQS, hex and rectangular geometry</td>
<td></td>
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<tr>
<td>CONcERT&lt;sup&gt;12&lt;/sup&gt;</td>
<td>1½-group CMDT, IQS</td>
<td>Used for training simulators</td>
</tr>
<tr>
<td>REMARK&lt;sup&gt;13&lt;/sup&gt;</td>
<td>Two-group course mesh finite difference equations</td>
<td>Used for training simulators</td>
</tr>
</tbody>
</table>
References


