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# Steady-state neutronics methods for power-reactor analysis

*Méthodes stationnaires en neutronique pour l'analyse des réacteurs de puissance*



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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Fax: +41 22 749 09 47
Email: copyright@iso.org
Website: www.iso.org

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# Foreword

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This document was prepared by Technical Committee ISO/TC 85, *Nuclear Energy, Nuclear Technologies, and Radiological Protection*, Subcommittee SC 6, *Reactor Technology*. This document is based on a standard developed by the American Nuclear Society (ANS) of which the current version is ANSI/ANS-19.3-2011 (R2017)[2].



 

# Introduction

The design and operation of nuclear reactors require knowledge of the conditions under which a reactor will be critical, as well as the degree of subcriticality or supercriticality when these conditions change. In addition, knowledge is required of the spatial distribution of neutron reaction rates in reactor components as a prerequisite, for example, for inferring proper power and temperature distributions to ensure the satisfaction of thermal-limit and safety-limit requirements. Both reaction-rate spatial distributions and reactivity can be and have been measured by suitable experimental techniques, either in mock-ups or in the operating reactors themselves. These quantities can also be calculated by various techniques. Available reactor experimental data have been used to validate the steady-state neutronic calculations within reasonable margins. As more accurate nuclear cross-sections become available and more refined calculation methods are developed, the reliability of the results of the steady-state power reactors will be considerably enhanced.

# Steady-state neutronics methods for power-reactor analysis

## 1 Scope

This document provides guidance for performing and validating the sequence of steady-state calculations leading to prediction, in all types of operating $UO_2$-fuel commercial nuclear reactors, of:

— reaction-rate spatial distributions;

— reactivity;

— change of nuclide compositions with time.

The document provides:

a) guidance for the selection of computational methods;

b) criteria for verification and validation of calculation methods used by reactor core analysts;

c) criteria for evaluation of accuracy and range of applicability of data and methods;

d) requirements for documentation of the preceding.

## 2 Normative references

There are no normative references in this document.

## 3 Terms and definitions

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

### 3.1 Terms

**3.1.1**
**application-dependent multigroup**
discrete energy-group structure that is intermediate between the application-independent multigroup structure and a few-group structure

Note 1 to entry: The application-dependent multigroup structure can be such that the group constants are dependent on reactor composition through an estimated neutron energy spectrum. An application dependent Multigroup data set is one type of averaged data set.

**3.1.2**
**application-independent multigroup**
discrete energy-group structure that is sufficiently detailed that the group constants may be considered as being independent of reactor composition, geometry, or spectrum for a wide range of reactor analysis

Note 1 to entry: The application-independent multigroup structure can be employed directly in reactor-design spectrum calculations, or it can be employed to generate group constants in an application- dependent multigroup structure. An application-independent multigroup data set is one type of averaged data set.

**3.1.3**
**cell**
one or more reactor sections with associated coolant (and possibly additional moderator and structural material) which, for computational purposes, are assumed to form a spatially repeating array in the reactor

Note 1 to entry: The simplest example of a cell is the "pin cell" in which a single fuel rod or pin is surrounded by coolant (e.g. light water, heavy water, or sodium). Another example is a bundle of fuel rods cooled by heavy water within a housing, surrounded by a heavy water moderator space.

Note 2 to entry: More complex geometric configurations are also used for some applications. These are often referred to as "supercells", or sometimes "(fuel) assembly cells", although the exact definition of the term varies greatly between reactor types and is even somewhat subjectively defined for a particular reactor type. Supercells, in the context of this document, represent more complex "cell" configurations which involve a collection of contiguous cells forming an assumed repeating array within the reactor, or augmented cells incorporating additional regions to serve as a computational artifice, e.g. to account for significant spectrum effects due to compositions outside the cell, or cell configurations including a reactivity device in addition to fuel, coolant, moderator and poison.

**3.1.4**
**data set**
collection of microscopic cross-sections and nuclear constants encompassing the range of materials and reaction processes needed for the application area of interest

**3.1.4.1**
**averaged data set**
data set prepared by averaging an evaluated data set or a processed continuous data set with a specified weighting function over a specified energy group structure

Note 1 to entry: The group structure and weighting functions may be selected to be application dependent. Application-independent averaged data sets for a wide range of reactor analysis, e.g. light water reactors, are dealt with in American National Standard Nuclear Data Sets for Reactor Design Calculations, ANSI/ANS-19.1-2002 (R2011)[1].

**3.1.4.2**
**evaluated data set**
data set which is completely and uniquely specified over the ranges of energy and angles important to reactor calculations

Note 1 to entry: Such a data set is based upon available information (experimental measurement results and nuclear theories) and employs a judgment as to the best physical description of the interaction process.

Note 2 to entry: An evaluated data set is intended to be independent of reactor composition, geometries, energy group structures, and spectra.

**3.1.4.3**
**processed continuous data set**
data set prepared by expansion or compaction of an evaluated data set using specified algorithms

Note 1 to entry: Such a data set is intended to be independent of reactor compositions, geometries, energy-group structures, and spectra.

**3.1.5**
**experimental data**
any experimentally measured quantity or quantities

Note 1 to entry: As such it is applied herein to both differential cross-section measurements and integral measurements (e.g. control-rod worth) obtained from reactor experiments or operations.

**3.1.6**
**few-group**
energy-group (typically 2-group) structure that is adopted for a particular application

Note 1 to entry: The few-group constants for a region are dependent on a specific reactor composition and geometry through a calculated energy spectrum, and are also dependent on temperature.

**3.1.7**
**lattice**
**lattice cell**
normally refers to a fuel-assembly cell with its associated immediate environment, such as the volume of moderator associated with it

**3.1.8**
**calculation method**
mathematical equations, approximations, assumptions, associated numerical parameters, and calculational procedures that yield the calculated results

Note 1 to entry: When more than one step is involved in the calculation, the entire sequence of steps comprises the "calculation method".

**3.1.9**
**reactivity**
property of the whole reactor, not just of a given material composition, is the ratio of the net production rate of neutrons (excess of neutrons produced by fission over those absorbed) to the production rate due to fissions

Note 1 to entry: Quantitatively, the core reactivity, $\rho$, can be represented as:

$$\rho = (\lambda - 1)/\lambda = 1 - (1/k_{\text{eff}})$$

where

$\lambda$ is the eigenvalue of the steady-state neutron balance equation;

$k_{\text{eff}}$ is the effective neutron multiplication constant.

Note 2 to entry: quantity (1 minus the eigenvalue of the steady-state neutron balance equation, written as:

$$M\Phi = \lambda F\Phi$$

where

$\Phi$ is the neutron flux;

$F$ is the neutron yield operator;

$M$ is the scattering, absorption, and leakage operator.

Note 3 to entry: The effective multiplication factor $k_{\text{eff}}$ is the inverse of $\lambda$. Reactivity is a unitless, pure number. It is, however, often written in terms of smaller "units", such as milli-k = 0,001, pcm = 0,000 01 = $10^{-5}$ or "dollars" (and cents), where 1 dollar is taken as the value of the delayed-neutron fraction in the system of interest.

**3.1.10**
**validation**
process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

**3.1.11**
**verification calculation**
process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model

## 3.2 Abbreviations

BWR boiling water reactor

HTGR high temperature gas cooled reactor

HWR heavy water reactor

LMR liquid metal reactor

PWR pressurized water reactor

# 4 Relation to other standards

The following American National Standards are related to this document:

— *Nuclear Data Sets for Reactor Design Calculations*, ANSI/ANS-19.1-2002 (R2011)[1], defines the criteria to be employed in the preparation of application-independent cross-section data files from experimental data and theoretical models. This document covers subsequent space and energy averaging processes which may be employed to prepare cross-sections for use in the representation of the core and its environment, and the subsequent calculation of the spatial distribution of neutron reaction rates in the core and of the core reactivity. There may be many ways of carrying out the space and energy averaging to obtain few-group cross-sections, and no unique path for the preparation or use of cross-sections employed in design calculations is defined, required, or recommended by this standard.

— *Guide for Acquisition and Documentation of Reference Power Reactor Physics Measurements for Nuclear Analysis Verification*, ANSI/ANS-19.4–2017[3]; and *Requirements for Reference Reactor Physics Measurements,* ANSI/ANS 19.5-1995; W2005[4].

Validation of calculation systems requires comparison with available integral experimental results. The preceding standards contain criteria for performing and documenting such experiments, in order to be most useful for this purpose.

— *Determination of Thermal Energy Deposition Rates in Nuclear Reactors*, ANSI/ANS 19.3.4–2002 R2017[5], provides criteria for the establishment of the thermal energy deposition rate distribution within a nuclear reactor core. Since the accuracy with which this can be done is dominated by the accuracy with which neutron reaction rates can be calculated, ANSI/ANS-19.3.4–2002; R2017 is closely related to ANSI/ANS–19.3–2011; 2017.

— *Quality Assurance Program Requirements for Nuclear Facility Applications*, ANSI/ASME-NQA 1 2015[6]. This standard deals with quality assurance, including that for computer programs.

— *Guidelines for the Documentation of Computer Software*, ANSI/ANS 10.3 1995 W2005[8]. This standard includes requirements for computer programs.

— *Verification and Validation of Non-Safety Related Scientific and Engineering Computer Programs for the Nuclear Industry,* ANSI/ANS-10.4–2008; W2016[9]. This standard deals with requirements or verifying and validating computer codes, such as those used for neutronics calculations.

— *Accommodating User Needs in Scientific and Engineering Computer Software*, ANSI/ANS-10.5–2006; R2016[10]. This standard deals with methods to respond to users' requirements in computer programs.



 

# 5 Methods of calculation

## 5.1 General

Calculations within the scope of this document would typically be performed in a sequence of steps. A typical sequence might be:

a) *Spectrum Calculation*. Averaged-data set cross-sections, nuclide number densities, and geometrical information (usually repeating cells or supercells) are used to calculate an application-dependent neutron spectrum for each different reactor region or composition.

b) *Cross-Section Collapsing*. Collapsing averaged-data set cross-sections to few-group form, using spectrum calculated in a) above.

c) *Cross-Section Homogenization*. The spectra obtained above are used to homogenize cross-sections and number densities over pin cells and assemblies.

d) *Flux Distributions and Reactivity*. The broad-group cross-sections and geometrical information about the reactor obtained above is used to calculate reactivity and few-group flux spatial distributions in the reactor.

e) *Reaction Rates Calculations*. The preceding information is used to compute reaction rates in physical reactor components.

f) *Exposure*. Calculation of changes in nuclide composition of fuel and possibly other reactor components with exposure are obtained based on the above data.

Not all steps in the sequence would normally be executed for a given problem. It is not a requirement of this document that a particular sequence of calculations, such as the one previously listed, be used. Similarly, the use of the preceding sequence does not, in itself, demonstrate compliance with this document. The use of a specific calculation procedure shall be justified by the procedure presented in Clause 6. However, the preceding sequence does provide an adequate framework within which most of the problems in steady-state reactor physics calculations can be discussed. Therefore, each of the aforementioned steps will be discussed in later passages of this subclause.

A summary of the requirements of this document is given in Clause 8.

## 5.2 Conditions to be considered

Consideration shall be given to all conditions which significantly affect the calculated quantities. The method of calculation shall be capable of treating the reactor composition or configuration under the conditions being studied.

Important conditions that may be significant include, but are not limited to:

a) presence of control elements (rods, cruciforms, or other forms), and degradation of the effectiveness of control elements;

b) presence and spatial distribution of burnable or soluble absorbers;

c) presence of adjacent, unlike fuel assemblies;

d) composition and geometric layout of fuel in an assembly;

e) dependence of coolant or moderator density upon conditions, or their spatial dependence;

f) depletion dependent conditions, including previous power history, coolant-density history, control-element history, and soluble-absorber history of fuel assemblies;

g) presence of materials or conditions, or both, outside the core, such as the core shroud in a BWR;

h) presence of sources, detectors, structural materials, and experimental devices;

i) spatial variations in temperatures;

j) fuel temperature;

k) spatial and temporal variations of important nuclides, e.g. xenon, samarium, and actinides.

## 5.3 Fine-group cross-sections

### 5.3.1 Basic data

The primary sources of basic nuclear data that are used for the generation of fine-group constants are evaluated data sets. Examples of these are the ENDF, JENDL, BROND, JEFF, and CENDL evaluated data sets. The properties and criteria for selecting these sources of basic nuclear data are specified in ANSI/ANS 19.1-2002 R2011[1].

### 5.3.2 Preparation of fine-group cross-sections

The preparation of application-dependent fine-group constants from existing application-independent fine-group constants shall entail use of an application-dependent energy spectrum estimate (see 5.3.3 and 5.4). This procedure employs a weighting spectrum that is selected to preserve important system-dependent characteristics during the averaging process. These characteristics usually include reaction rates, and may include other quantities.

### 5.3.3 System dependent spectrum calculations

The fine-group cross-section set (5.3) should be used in the calculation of the neutron energy spectra in the system under investigation. The energy spectra are established by the geometry, material composition, and the operating conditions of the reactor in an interplay of neutron leakage with reactions such as absorptions and scattering. The neutron energy spectrum may vary from one region of the core to another and it may be necessary to compute the spectra for several representative regions of the reactor core.

### 5.3.4 Weighting function

The fine-group constants can be sensitive to the selection of an energy dependent weighting spectrum, and to the choice of group structure. The smaller the number of energy groups, the greater the sensitivity will be. Therefore, an estimate of the reactor spectrum is needed and should be obtained from measurements in identical or similar reactors, or from analytical models of neutron slowing down or source spectra. It should be noted that results may be sensitive to the modelling of the spectra and the choice of group structure.

## 5.4 Preparation of broad-group libraries

### 5.4.1 General

There are three distinct steps for generating broad-group libraries:

a) processing of continuous or point-wise cross-sections, accounting for self-shielding and Doppler broadening effects and collapsing these data into a fine-group library using an appropriate spectrum;

b) performance of fine-group transport calculation for a simplified model of the reactor to obtain a fine-group spectrum;

c) utilization of the fine-group spectrum to obtain broad-group libraries.



 

### 5.4.2 Choice of cell and supercell

Many reactor cores can be thought of as composed of repeating units called cells, such as a single fuel pin cell or a fuel assembly cell (e.g. sometimes this formalism is extended to absorber pins or water holes), with its associated structures, coolant, and moderator (where this is distinct from the coolant).

Once a cell is selected, one approach is to compute the spectrum representative of this cell. It is necessary to inspect the cell and its surroundings to determine if the spectrum in the cell is generated by the cell and its similar surroundings alone, or if the spectrum in the cell is influenced by parts of the reactor not made of similar cells. When the spectrum is influenced by regions of the core external to the cell, a supercell may be defined, and the spectrum characteristic of the supercell is computed. The supercell may be a repeating unit of the reactor containing non-cell materials such as water channels, control-rods, and structural materials. Other non-cell regions such as absorber pins, when present, should be included in the supercell if they significantly influence the spectrum. For either a cell or a supercell, outer boundary conditions are specified consistent with symmetry assumptions.

### 5.4.3 Cell environment

The assumption that a reactor is made of an array of similar cells or supercells is, at best, an approximation, and if the spectrum in the cell is influenced by external regions, these effects should be included in the spectrum calculations. These effects may be caused by leakage across the cell or supercell boundaries, and thus may be energy and direction dependent. Temperature effects in fuel, in moderator or coolant, or in both (e.g. Doppler broadening), and variations in density of coolant or moderator, or both, shall be included in the calculation. Corrections for a non-uniform temperature distribution within the cell and supercell should be made, or the temperature distribution should be included in the calculation.

### 5.4.4 Calculation model

The calculation model often can be considered to consist of two parts, the geometric model and the neutronic transport model, though the two parts may not be clearly separable.

#### 5.4.4.1 Geometric model

The geometric model refers to the manner in which the physical configuration of the cell is represented in the mathematical solution. Geometric approximations may be employed when all aspects of the physical configuration are not of comparable importance, the primary objective being to reduce the number of dimensions employed in the solution of the problem or to transform to a more convenient or simplified geometry. Different geometric approximations may be made concerning the same physical configuration for different purposes. The choice of geometric models appropriate to the analyses shall be justified and documented.

In some calculations, one geometric dimension of the model may be dropped, as long as the leakage in the missing direction is taken into account by the judicious inclusion of a buckling term which stands as the surrogate of the missing leakage.

#### 5.4.4.2 Neutronic transport model

Various calculation procedures may be utilized to describe neutron transport phenomena in cell studies. Different degrees of approximation may be made depending on the nature of the problem and the objectives of the calculation. There are two basic approaches in modelling neutron transport in power reactors: deterministic and Monte Carlo. Various deterministic methods are used, such as collision probability, discreet ordinates and nodal diffusion methods. A very detailed type of calculation is continuous-energy Monte Carlo. This statistical procedure follows “histories” of large numbers of individual neutrons. Initially, this technique served primarily as a guide to the validity of other (deterministic procedures) but is now used in mainstream applications as well.

Deterministic transport models generate numerical solutions (by collision probability methods, for instance) of the integral transport equation. Approximations may also be introduced in representing

energy-transfer kernels. The analyst shall demonstrate and document that the transport model used is appropriate to the problem under consideration. For example, in using discrete ordinate methods, the analyst shall show that the spatial mesh, the order of scattering (P1, P3, etc.), and the order of quadrature (in Sn methods) are adequate to achieve stated accuracy levels for the calculated reactivity and reaction rates.

## 5.5 Collapse to few-groups

When performing full reactor calculations it is usually adequate and desirable to collapse the cross-sections from the fine-group structure into a broad-group set. The actual group structure chosen should depend on the type of calculation and the sensitivity of that calculation to the group structure.

When collapsing cross-sections to a broad-group, important system characteristics – such as reaction rates in a unit-cell, reactivity of the cell and core, or reaction-rate ratios – should be preserved. This preservation is an attempt to maintain some of the detailed representation of the fine-group calculation in the coarser broad-group calculation. The actual quantity or quantities preserved and the method of doing this should depend on the intended use of the few-group data.

The calculation used in the collapse shall include or account for all important effects of space and energy that cannot be adequately modelled in the calculations to follow, such as self-shielding and spectrum dependence on surrounding materials.

The cross-sections of each nuclide present, to a significant degree, shall be retained individually whenever calculations of individual reaction rates are to be carried out. These cross-sections should also constitute the starting (reference) points for calculations of change in nuclide composition with time (depletion calculations).

## 5.6 Calculation of reactivity, reaction rate, and neutron flux distributions

### 5.6.1 Models

The calculations being considered in this section have as their objective the computation of a measure of closeness to criticality of a specified reactor-core configuration, and the reaction rates as a function of position in the core under steady-state or quasi steady-state condition. A number of models may be used for this purpose.

A frequently used measure of closeness to criticality is the effective multiplication factor ($k_{\text{eff}}$). This is appropriate, for example, in describing the closeness to criticality of a reactor in its shutdown condition. However, most steady-state reactor calculations are intended to represent conditions at critical or an artificial steady-state for the purpose of calculating reactivity margins or reactivity coefficients. Under these circumstances, a value of $k_{\text{eff}}$ different from unity represents an artificial device. In addition, code-system bias and uncertainties may lead to a non-unity $k_{\text{eff}}$ as a critical reference point. The definition of reactivity in this document is then $[1-(1/k_{\text{eff}})]$.

For the purpose of discussion in this subclause, it is assumed that cross-sections for all regions of the reactor have been generated in fine-group or broad-group homogenized form by the techniques described previously. A number of models are in common use for performing neutron-flux calculations. Some of these are:

a) solving the diffusion equations by finite-difference, finite-element, or synthesis methods;

b) solving the transport equations by discrete-ordinates or collision-probability methods or by the method of characteristic;

c) solving the reactor neutron balance equations by nodal diffusion methods;

d) the continuous-energy Monte Carlo method with spatially detailed representation and large number of neutron histories, provides a superior alternative to deterministic methods.



 

The preceding examples of models are by no means exhaustive of models that may be used. However, they are sufficient to illustrate the variety of methods being used, each of which may have characteristic types of uncertainties and assumptions.

### 5.6.2 Uncertainties and assumptions

In setting up a computer model of the reactor core intended to simulate steady-state neutronic behaviour (core-follow or predictive analysis), certain assumptions and simplifications are usually made. Depending on the number and extent of simplifications and the number of assumptions, each of them can result in errors which are cumulative. Therefore, the results of the calculations can only be considered as approximate.

For example, it may be assumed that the neutron flux or current remains constant over small areas or along small line segments. Thus, the solution produced by the computer program will be an approximation to the solution of the model equations.

The following are examples of many modelling assumptions or approximations that are commonly made, and which may contribute to a calculation bias and/or to uncertainties:

a) the assumption that neutron flux in the core as a function of all three spatial dimensions may be represented as the product of functions which separately are a function of only one or two dimensions (spatial separability);

b) geometrical transformations used to model the physical situation;

c) the use of artificial boundary conditions within the core (e.g. at the boundaries of heavily-absorbing control slabs or cruciforms);

d) assumptions of symmetry for configurations which are not precisely symmetric;

e) the choice of a small number of energy groups to represent the neutron energy variation in the core;

f) the assumption of linearity of flux between the spatial points within a spatial mesh structure, the dimensions of which may be specified somewhat arbitrarily;

g) the use of bucklings to simulate leakage effects in the directions are not explicitly represented;

h) the assumption that dissimilar media may be homogenized;

i) the use of pre-calculated region-homogenized (typically lattice-homogenized) cross-sections at a predefined power history;

j) the use of interpolation or curve fitting technique for the calculation of cross-sections at local conditions.

All of the preceding assumptions or approximations are, in principle, amenable to numerical studies aimed at establishing the deviation of the normally used procedures from more precise solutions of the model equations. Numerical methods should normally be used only within the range of parameters for which the biases or uncertainties of the methods are known. When stepping outside this range, caution should be exercised to try to ensure that there are no fortuitously cancelling error, and to be in a better position to judge the reasonableness of the behaviour of the method and of the results obtained.

## 5.7 Calculation of reaction rates in reactor components

When a model which simplifies the physical description is used, means shall be provided to convert the results of the model calculation into reaction rates in the physical components as required by the application. If the calculation procedures make use of simplifying assumptions, such as separability of local and overall flux variations, the procedure shall specify how local reaction rates are obtained, and the basis or justification for the technique employed shall be described.

The reaction rates thus calculated are used for a variety of purposes. Some examples are:

— computation of heat generation rates for heat transfer and thermal hydraulic calculations, which, in turn, are used to verify thermal limits;

— computation of change in nuclide composition of fissile-nuclide-bearing materials as a function of position in the core in order to predict fuel inventory;

— computation of shutdown margins, control-rod worths, and reactivity worths of other components;

— computation of the relationship between detector response and in core reaction rates.

## 5.8 Depletion calculations

In a critical reactor, the rate of change in the concentration of a nuclide is the difference between the rate of production of that nuclide and the rate of destruction of that nuclide. The most significant production mechanisms are neutron capture in the transmutation precursor, the decay of another nuclide, and direct fission yield (in the case of fission products). The most significant destruction mechanisms are fission, neutron capture in the nuclide, (n, xn) reactions, and decay of the nuclide. Yields of fission products, including lumped pseudo fission products, and decay constants of the nuclides of interest are basic nuclear data which shall be available to any such calculation.

One common procedure is to assume that the supercell representation (or lattice calculation) and associated neutron flux spectrum have adequate accuracy to allow depletion calculations. The neutron spectrum is used in summing the product of the cross-sections and fluxes into total fission, capture, and (n, xn) reaction rates. These, together with the fission yields and decay constants, provide the production and loss terms for each nuclide. The result is a set of coupled differential equations for the concentration of all nuclides of interest. These equations are solved simultaneously by numerical methods, through the use of discrete time steps. The equations may be reduced to linear equations, since this is appropriate to the solution technique. The time steps shall be set sufficiently small to ensure numerical stability of the solution technique and accuracy appropriate to the application. It is also necessary to ensure that the flux level in depleting regions does not rise so rapidly that the required time step length becomes exceedingly short. In such cases the numerical solution method shall include estimates of the variation of the flux level within the chosen time step length.

In order to lengthen the permissible time step, it is common practice to assume that some nuclides with very large decay constants are in equilibrium at all time steps. The choice of these nuclides may be under the control of the analyst. If so, the choice should be made consistent with the intended applicability of the results.

Fission, capture, and (n, xn) reaction rates near the beginning of exposure are normally obtained from the zero exposure cross-sections of all nuclides of interest. As the depletion calculation proceeds from zero exposure, concentrations change and group averaged cross-sections may change as a result. Both spectrum changes and changes in resonance self-shielding factors contribute to these cross-section changes. Thus, it may be necessary to recalculate the supercell spectra with updated concentrations at intervals in order to obtain group averaged cross-sections and other parameters such as diffusion coefficients as a function of time, exposure, number density, etc.

The interval between supercell spectrum calculations is normally under the control of the analyst. The form in which this can be specified may vary; e.g. fuel exposure interval, or percent change in concentration of a specified nuclide (usually $^{235}U$). The procedure for selecting a satisfactory interval is straightforward. The interval is reduced in successive calculations until the differences in concentrations are insignificant for the intended application. This procedure shall be used in the absence of established criteria which can be justified for the application.

The few-group cross-sections obtained from the supercell calculation may be used to perform a spatial reactor depletion calculation. The cross-sections may be calculated as functions of exposure, nuclide concentrations, and/or other variables (such as moderator density and temperature, fuel temperature, void fraction, and controlled state) or may be retained as functional fits to or as tabular data with interpolation and extrapolation.



 

The preceding discussion is applicable if it has been judged that the supercell representation and spectrum has adequate accuracy to allow proceeding to depletion calculations through the use of macroscopic cross-sections.

This assumes that the number-density ratios will not change with time as the core depletes with locally and possibly globally varying power level, moderator temperature, void distribution, etc.

If this cannot be justified, a more accurate approach shall be used. The supercell calculation is used to generate few-group cross-sections as a function of exposure, nuclide concentrations, and/or other variables, which are retained for use in the few-group reactor core calculation. The depletion equations may then be solved as before, or individually for each explicit nuclide. In the first case the macroscopic cross-sections shall include dependence on separately defined history variables, such as power level, moderator temperature and density, fuel temperature, $^{135}Xe$ concentration, etc.

This procedure will produce different results to the extent that the few-group spectra from the reactor calculation differ from the few-group spectra in the supercell calculations.

## 5.9 Common practices

Experience with PWR, BWR, HWR, HTGR, and LMR reactors is sufficiently extensive that a set of common practices has been developed for each. General descriptions of these practices are given in the following passages. The fact that a particular reactor or reactor type is not included in these passages does not imply that the methods used in its design or operation do not fulfil the requirements of this document. The requirements of this document are delineated in Clause 8.

The accuracy of the various models can be checked against measurements or against the results of fundamental techniques such as Monte Carlo.

### 5.9.1 Pressurized water reactor (PWR) core physics method

There are in general three distinct steps in steady-state PWR reactor physics analysis: library generation, assembly lattice calculations, and reactor core calculations. The purpose of these calculations is to provide the basis for reactor core design, including safety and economic evaluations. Figure 1 illustrates the sequence of such analyses and their relationships to each other.

Reactor physics analysis begins with continuous-energy cross-section or fine-group libraries and other nuclide data which have been generated by the processing of data from a version of an evaluated data set, such as the Evaluated Nuclear Data File (ENDF/B), of which ENDF/B VI[11] and ENDF/B-VII[12] are recent examples, the Joint Evaluated Fission and Fusion Library (JEFF)[13] produced by the NEA Joint Evaluated Fission and Fusion project, of which JEFF-3.1.1[13] is the current version, the Russian Library of Evaluated Neutron Reaction Data (BROND)[14] or the Japanese Evaluated Nuclear Data Library (JENDL)[15]. These multigroup libraries typically contain 40 to 200 energy groups with tables of thermal cross-sections and resonance integrals as function of temperature and dilution cross-sections. Libraries may also contain the probability table parameters. Thermal cross-sections are generated through the use of a “generic” PWR spectrum. The cross-sections in such libraries may or may not have been modified subsequent to the processing from evaluated data in order to improve agreement between downstream models (lattice and nodal models) and measurements. These libraries, as shown in Figure 1, provide the basis for the fine-group lattice physics calculations.

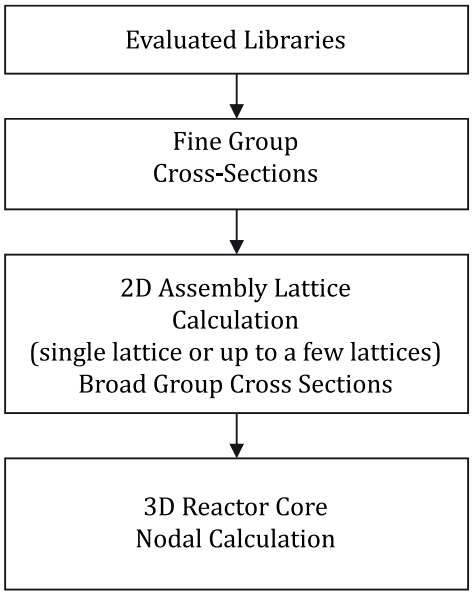


**Figure 1 — General flow of data for PWR physics calculations**

### 5.9.2 Boiling water reactor (BWR) core physics methods

There are in general three distinct aspects of BWR reactor physics analysis: library generation, lattice calculations, and nodal calculations. Figure 2 illustrates the sequence of such analyses and their relationship to each other. The general sequence of BWR calculations is the same as for the PWR counterparts, although the calculations differ in some particulars. Most of the application independent fine-group libraries for BWR applications are generated by processing data from a recent version of an evaluated data set, such as the Evaluated Nuclear Data File (ENDF/B-VI[11] or ENDF/B-VII[12]). These libraries typically contain 40 to 200 fine-groups. The nuclide cross-sections within a specific group structure are processed through the use of a "generic" BWR energy spectrum. These libraries, as shown in Figure 2, provide the cross-section data for fine-group lattice-physics calculations.

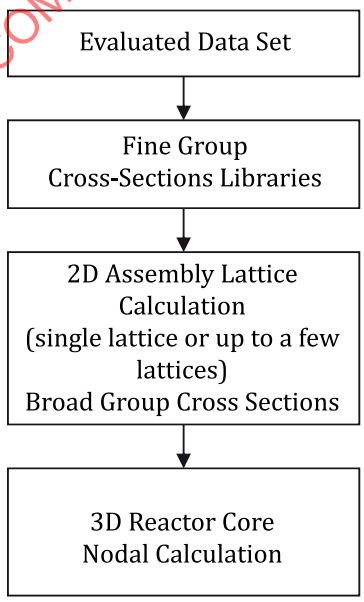


**Figure 2 — General flow of data for BWR physics calculations**

BWR fine-group lattice-physics calculations typically are two dimension transport theory calculations that employ a fine spatial mesh. They usually are performed for a single lattice, although they may



 

involve several lattice cells for special-purpose applications. These calculations have three separate but complementary components: fine-group pin-cell calculations, intermediate-group lattice calculations, and nuclide depletion calculations. Initially, fine-group thermal and epithermal calculations are performed for the individual fuel pins or fuel-pin types and water rods or water holes, and structural components within the lattice, respectively. Fuel rods containing integral burnable poisons are usually modelled in greater detail and/or with more precise methods. These fine-group calculations typically employ the same energy group structure as the cross-section library. The pin cells then are homogenized, and intermediate-group cross-sections for the homogenized cells are edited from the results of the pin-cell calculations. Next, intermediate-group calculations are performed for the lattice as a whole, with each homogenized pin cell retaining its own identity. Usually, both the pin-cell calculations and the intermediate-group calculations are based on transport theory. The number of energy groups in the intermediate-group calculation may range from as few as half a dozen to as many as are present in the library. Broad-group cross-sections then are edited from the intermediate-group calculation for a homogenized representation of the lattice. Finally, nuclide depletion calculations are performed for those nuclides whose concentrations change with time, including lumped pseudo fission products. More sophisticated methods are required to calculate burnable-absorber depletion properly.

The cross-sections edited from the intermediate group calculations are used as input to nodal calculations. Consequently, different sets of intermediate group calculations are performed for different combinations of thermal-hydraulic variables, fuel exposure, nuclide decay (e.g. shutdown time), and control-rod state. The values of individual variations generally are chosen so that they span the range of conditions expected to be encountered during core operation.

Nodal core calculations are performed for three-dimensional homogenized core analysis. Individual bundles are divided into stacks of homogenized nodes, each of which typically is 10 to 30 cm high. Nodal calculations are based on diffusion theory. Although effective one-group nodal models that preserve the fundamental-mode multiplication factor ($k_{eff}$) of two-group or three-group nodal models are still in use, many now employ two or three-group advanced nodal models for this purpose. The nodal codes shall account for significant thermal-hydraulic feedback into their cross-sections and may include explicit nuclide depletion for actinides, major fission products, and burnable absorbers within the node. However, most current codes use “macroscopic” depletion models (macroscopic cross-sections parametrized as functions of exposure, instantaneous void fraction, void-fraction history, fuel temperature, control-rod presence and control history) and treat nuclide behaviour of only $^{135}$I, $^{135}$Xe, and (perhaps) $^{149}$Pm and $^{149}$Sm explicitly.

Feedback effects between local power and moderator density (void) are prominent in BWRs. Consequently, the flow distribution for the reactor core calculation, whether input or internally calculated, should correspond to a condition where the core pressure drop is the same for all parallel flow channels. It is important that all pressure drop effects and local void formation be accurately modelled. These variables strongly influence the reaction-rate distributions and reactivity of the core.

### 5.9.3 Liquid metal reactor (LMR) core physics methods

The steps for carrying out the reactor physics analysis of an LMR are illustrated by the flow diagram shown in Figure 3. This diagram resembles those for light water reactors. However, greater detail needs to be included in the energy structure used for the reactor calculations, as the essential reactions occur in a wider energy range and as the energy spectrum changes significantly with design detail and spatial location in the core.

The generation of fine-group cross-sections from a nuclear data file such as ENDF/B-VI[11] or ENDF/B-VII[12] serves as the starting point for LMR analysis. Fine-group constants are commonly generated for a fine energy-group structure (50 to 250 energy groups) through the use of one of two different approaches.

In the first (or “ultrafine-group”) approach, “smooth” cross-sections for a very fine energy structure (2 000 or more energy groups) are first processed from the ENDF data by averaging the cross-sections in each small energy interval. The broad structural resonances are explicitly represented in the “smooth” fine-group constants, while the narrow resonances are excluded and treated separately. Infinite-medium fine-group spectra are then computed for the very fine energy structure through the use of

representative fast reactor compositions; the resonance reaction contributions are evaluated using the narrow resonance (NR) approximation. Fine-group cross-sections are then generated through the use of the detailed smooth reaction rates and resonance reaction rates, along with the detailed energy spectrum.

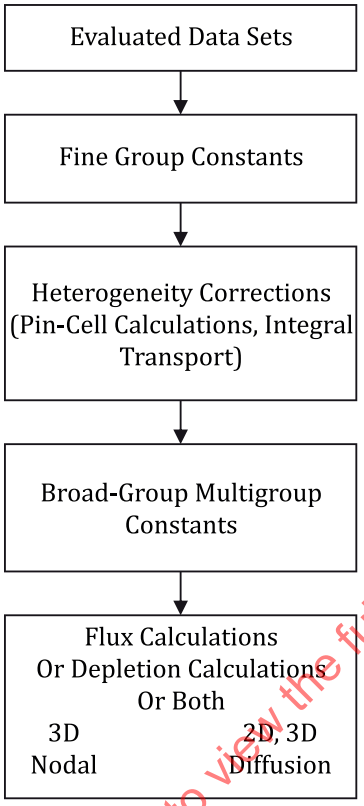


**Figure 3 — General flow of data for LMR physics calculations**

In the second approach, fine-group cross-sections for a particular application are generated through the use of the shielding factor methodology. This method utilizes an application-independent master cross-section library, as described in ANSI/ANS 19.1 1983 (R2002)[2]. Such a cross-section library contains both group-averaged cross-sections (averaged over a representative fast reactor spectrum) and tables of group-¬dependent resonance self-shielding factors, which together are used to prepare cross-sections that are properly resonance self-shielded, for specific conditions of interest. The data are normally provided in a group structure of 50 to 250 energy groups. The resonance self-shielding factors for each resonant isotope and each energy group are normally provided in table form as a function of the concentration of the resonant isotope (represented by the background cross-section) and its temperature. These shielding factor data are combined with the "unshielded" (infinitely dilute) cross-sections by a cross-section preparation code which calculates the appropriate background cross-sections for each reactor region and performs the table interpolation to obtain the appropriate resonance self-shielding factors.

Because the neutron mean free path is large compared to the small pin diameter in most fast reactor systems, heterogeneity effects are of relatively minor importance. However, heterogeneity corrections are commonly applied to the multigroup cross-sections for the appropriate assembly design. For a given pin-cell geometry, heterogeneity effects are generally evaluated in the "ultrafine-group" approach through the use of an integral transport calculation on a fine energy mesh. In the shielding-factor method, heterogeneity effects on resonance shielded cross-sections are commonly incorporated based on equivalence theory during the preparation of application dependent cross-sections for a specific composition and temperature.

Broad-group cross-sections appropriate to the various reactor regions are ordinarily generated by collapsing the fine-group cross-sections (prepared by either of the two methods above) through the use

of neutron energy spectra obtained from one or more spatial calculations. The collapsing calculation utilizes a neutronics model in which representative reactor materials are placed in a simplified configuration. Broad-group cross-sections are generated for multiple spatial regions where the material compositions and neutron energy spectrum remain roughly constant.

Reactor calculations, of reactivity effects, neutron reaction rates, and flux distributions, are performed with three-dimensional nodal (or finite difference) diffusion theory methods; assemblies are radially homogenized; and corrections for transport effects are sometimes obtained from two dimensional transport codes in r z, x y, or triangular geometries. Three-dimensional transport codes (deterministic and Monte Carlo) are also being utilized with increased frequency for LMR analysis.

The fuel depletion calculations are carried out through subdivision of the burn cycle into one or more subintervals, and performance of an explicit depletion calculation in each region of the reactor over each subinterval through the use of average reaction rates over the subinterval. These average reaction rates are based on three-dimensional fluxes calculated at both the beginning and end of the subinterval. The nuclide transmutation equations are solved explicitly. The isotopes to be considered in the depletion equations, as well as their transmutation reactions, are specified by the analyst. The depletion calculations are performed for radially homogenized models of the assemblies; pin wise power densities and nuclides are usually "reconstructed" by interpolation of assembly wise quantities.

### 5.9.4 Heavy water reactor HWR core physics methods

A generic model for HWR (CANDU) reactor analysis is shown in Figure 4. Reactor physics analysis begins with fine-group, microscopic cross-sections or with cross-sections based on analytical spectra and with other nuclide data which have been collected into one or more cross-section libraries. These libraries usually have been processed from extensive tabulations (e.g. the Evaluated Nuclear Data File/B (ENDF/B) (see Reference [12]). The cross-sections in such libraries may have been modified subsequent to processing from evaluated data in order to improve agreement between measurements and results computed by downstream lattice models. The general methodology for CANDU reactor physics calculations is a 3-step process:

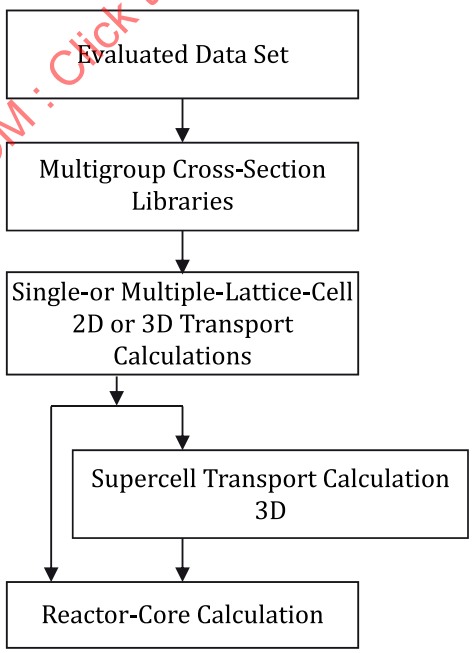


**Figure 4 — General flow of data for HWR (CANDU) physics calculations**

a) The first step consists of lattice calculations for the bare lattice, i.e. for basic unit-cells containing fuel, coolant, pressure and calandria tubes and the surrounding moderator volume, but excluding the representation of any interstitial reactivity devices. The lattice calculation is usually performed for a single cell (or sometimes for multiple lattice cells) in 2 (or sometimes 3) dimensions with a

transport theory code. It is usually carried out in a detailed geometrical model, with a detailed representation of the flux spectrum, and for all relevant lattice conditions, such as: fuel depletion; fuel, coolant, and moderator temperatures; and densities; etc. In performing lattice calculations it is normally necessary to repeat the lattice spectrum calculation at different burnups in order to account for the effect of changes in nuclide inventory. The lattice calculation provides homogenized properties for the cell (or for each cell in a multiple-cell configuration) in a few (usually two) energy groups, for input to the finite-core calculation.

b) The second step consists of supercell calculations in three dimensions, to determine the effect of interstitial reactivity devices on homogenized properties in their vicinity. This effect is cast in the form of few-energy-group (usually two-energy group) "incremental" cross-sections, which are to be added to the bare-lattice cross-sections (calculated in step a) of cells traversed by a reactivity device. Supercell calculations are performed with a transport theory code, and usually in 3 dimensions, because CANDU reactivity devices are perpendicular to the fuel channels. The device incremental cross-sections are determined by performing two supercell calculations, one with the device included in the model, and another with the device excluded, and subtracting the homogenized cross-sections obtained in the two cases.

c) The third step is the three-dimensional-diffusion-theory calculation for the entire core, using 2 or more energy groups. In this calculation, the finite-reactor model is obtained by superimposing the lattice cross-sections obtained in the first step and the device incremental cross-sections obtained in the second step. The finite-reactor code calculates the core eigenvalue and the global distribution of flux and power. The fuel at different positions in core has a different value of fluence, and its properties are evaluated as a function of its fluence in a snapshot or core-follow calculation, or are fluence-averaged in the time-average (equilibrium) core model.

For an accurate calculation of the power distribution in the HWR (CANDU or Advanced CANDU reactor), it is important to generate cross-sections for each fuel bundle in the core, accounting for local conditions (fuel temperature, coolant density, moderator purity, etc.) and the burnup history of the fuel bundle, as well as the effects of the environment if necessary. Different approximations can be used to treat the local parameters and their history in the CANDU or Advanced CANDU reactor core and to provide lattice properties corresponding to an instantaneous state of the core.

The simplest technique is the uniform-parameter method. In this method, the lattice properties are functions of fuel burnup only, by assuming effective core-average conditions for each fuel bundle. An improved approach is the local-parameter method (also called the macro-depletion method in LWR applications). In this approach, the lattice properties are functions of fuel burnup and other local parameters. Since the macroscopic cross-sections used in the interpolation are generated beforehand at various assumed operating conditions, this method does not take into account the dependence of the cross-sections on a bundle's history. A more accurate approach, the micro-depletion method, has been developed and used for the CANDU or Advanced CANDU reactor. This method is as simple as the macro-depletion method but it tracks both the microscopic cross-section of a nuclide and its number density, which depends on the depletion history.

A more rigorous method is the history-based local-parameter method developed for HWR (CANDU). This is recognized as the most accurate way to calculate the evolution of nuclear properties, but is not always performed, depending on the lattice code used.

In this method, the lattice code is coupled directly with the core-analysis code, and the lattice calculations are performed for each bundle at each time step, so as to treat local parameters and the history of each bundle individually. This method relies, in practice, on the assumption that the lattice properties associated with a given reactor state can be calculated (perhaps directly within the core-analysis code) with a simplified lattice-cell code with only a few energy groups. While it would be desirable to use lattice properties from a modern lattice-cell code directly for history-based local-parameter calculations in the core-analysis codes, this is still impractical for routine calculations at this time, because of the computational effort required.

The homogenized lattice properties are usually performed for a single lattice cell (considered as the heterogeneous medium) with reflective or periodic boundary conditions, without considering the effect of the environment. In some cases, multiple lattice cells (multicells) can be used to correct for



 

the effect of the neighbourhood on a single lattice cell or the effect of the presence of the reflector. The multicell methodology, developed for the CANDU or Advanced CANDU reactor, maintains intact the basic structure of the single-lattice-cell based micro-depletion method.

The accuracy of the HWR lattice and core calculations may be checked by comparison with measurements or against results of other fundamental methods, such as Monte Carlo methods.

### 5.9.5 High temperature gas cooled reactor (HTGR) core physics methods

The HTGR model outlined in Figure 5 illustrates, in summary fashion, the general steps in the sequence of design codes used in the physics analysis for HTGRs. The primary result being sought is the time dependent behaviour of the core power and flux distribution throughout the life of the reactor core. Data are also produced on nuclide concentrations as a function of depletion, control-rod reactivity worth, core shutdown margins, core reactivity, reactivity coefficients, and core kinetics parameters.

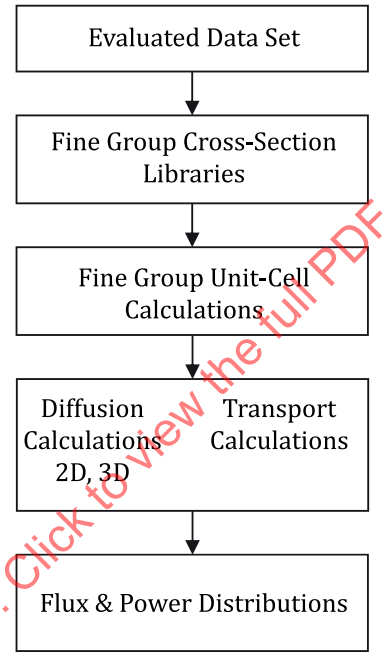


**Figure 5 — General flow of data for HTGR physics calculations**

Reactor physics analysis begins with cross-sections collected into fine-group libraries (see References [1] and [12]). These libraries have been processed from extensive tabulations of basic, evaluated cross-section data such as the Evaluated Nuclear Data File/B (ENDF/B). Generally, the most recent evaluation is used.

The calculation sequence is similar to the models used for LWRs. Unit-cell calculations or lattice (assembly) codes, which read the fine-group libraries, are used to generate few-group (also known as broad-group) cross-section data sets. The few-group cross-sections form the starting point for multidimensional reactor core calculations. Because the fuel is in the form of coated particles in HTGRs, particle self-shielding is important and is usually accounted for in the unit-cell calculations.

The broad-group cross-section data are used in combination with geometric, fuel loading, and operational data for performance of the physics analysis. Typically, this analysis may start with simplified, often point reactor, calculations and then proceed to two- and three-dimensional finite-difference or nodal methods for solution of the diffusion equation in the reactor core geometry. Design problems for which transport theory is required include determination of flux disadvantage factors, boundary conditions for control-rods and burnable absorbers, and other situations involving anisotropic scattering or strong neutron absorption or leakage.

Depletion of fuel, fertile material, burnable absorbers, and fission products is calculated throughout the reactor core lifetime and with sufficient spatial resolution. Typically, basic point reactor fuel-cycle studies provide rapid determination of fuel loadings followed by two- and three-dimensional depletion studies. Core leakage in the depletion calculations is modelled by a group dependent leakage correction to the fission source term to reduce the error due to spectrum changes with depletion. Cross-section variations with time and temperature are accounted for as necessary.

# 6 Verification and validation of the calculation system

## 6.1 Overview

Verification and validation are two complementary aspects in determining the range of applicability of the calculation system. As defined in 3.1, verification assesses the fidelity of the calculation system to the theoretical models upon which it is based, while validation assesses the accuracy with which the calculation system predicts real-world behaviour. A simple example of verification is the determination of the accuracy with which a diffusion theory code produces solutions to the neutron diffusion equation, irrespective of whether diffusion theory is an appropriate representation for the behaviour of interest. An example of validation is the comparison of the calculation system's predicted value for, say, the core power distribution with the distribution that was actually measured.

The components of the calculation system shall be tested both individually and collectively. Testing of a single component is referred to as unit testing, while testing of the system as a whole is referred to as integral testing. The components of the calculation systems employed for core reactivity and power distributions for most power reactors generally fall within one of four general categories:

a) nuclear data;

b) lattice codes (and supercell codes, if applicable);

c) linkage codes;

d) reactor core codes.

Although these categories are not universal, extension to those types of reactors that have additional components should be straightforward.

Unit testing of nuclear data will not be discussed herein, as it falls outside the scope of this document. The interested reader is referred instead to Reference [1].

## 6.2 Verification

### 6.2.1 General

Verification typically involves comparisons with closed-form analytic solutions or reference results from a previously verified code. Verification is typically performed by the code developer, with the results included within the documentation distributed with the code.

### 6.2.2 Unit testing

#### 6.2.2.1 Overview

Analytic and/or simplified artificial benchmarks are the primary tool employed for unit testing within the context of verification. In general, verification is a binary process: the code either replicates the reference result to an acceptably fine level of precision or it does not. If it does not, the coding shall be examined until reasons for discrepancies are identified and understood. If these reasons are found to be one or more errors in the code, the code shall be revised, and the verification process shall be repeated.



 