MCB: A CONTINUOUS ENERGY MONTE CARLO BURNUP SIMULATION CODE

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Abstract

A code for integrated simulation of neutronics and burnup based upon continuous energy Monte Carlo techniques and transmutation trajectory analysis has been developed. Being especially well suited for studies of nuclear waste transmutation systems, the code is an extension of the well validated MCNP transport program of Los Alamos National Laboratory. Among the advantages of the code (named MCB) is a fully integrated data treatment combined with a time-stepping routine that automatically corrects for burnup dependent changes in reaction rates, neutron multiplication, material composition and self-shielding. Fission product yields are treated as continuous functions of incident neutron energy, using a non-equilibrium thermodynamical model of the fission process. In the present paper a brief description of the code and applied methods are given.

Introduction

Currently, the Monte Carlo transport code MCNP developed at Los Alamos National Laboratory is regarded as state of the art in the reactor neutron transport field [1]. Other codes are either benchmarked against MCNP (e.g. CASMO and ERANOS), or are not validated in the same respect as MCNP is (e.g. CERN's EET Monte Carlo code). Since MCNP itself does not calculate nuclide density evolutions, simulations of burnup in a material subject to intense neutron irradiation has until now been made by using simplified integrated transport and burnup codes like BISON, or by linkage of advanced neutronics codes as MCNP and ERANOS with specialised burnup codes like CINDER90, ORIGEN2 and DARWIN. The exception is the general particle transport and burnup Monte Carlo code developed by the EET-group at CERN, which however has not yet been made available for independent evaluation.

Such coupling of codes leaves the field open for inconsistencies on form of basic data discrepancies. It further sets high demands on the user capability of assigning time stepping grids adequate for spectrum changes and self shielding effects to be correctly modelled. Especially in the field of nuclear waste transmutation, where correct prediction of minor actinide and fission product density evolution of are of much higher significance than in simulations of commercial nuclear power plants, there is a need for better modelling tools. Hence it was undertaken by the present authors to extend the most advanced and best validated code for neutron transport available - MCNP - with advanced nuclide density evolution capabilities, including transmutation trajectory analysis, in order to create a fully integrated, well validated Monte Carlo Burnup simulation code - MCB.

Requirements

The requirements of the code development are set by the demand of a correct modelling of critical and sub-critical waste transmutation systems. These are supposed to transmute extraordinary large fractions of original materials present in the system. For instance, resulting material compositions after 20% heavy atom burnup and up to 50% long lived fission product transmutation during a single irradiation cycle must be correctly predicted by the code, which means that significant spectrum changes and self shielding effects have to be accommodated for. Further, in order to optimise fuel and waste management, it is advantageous to apply the transmutation trajectory analysis method, which provides additional information of the transmutation process, as compared to the exponential matrix method.

Implementation

Physical Data

The basic cross section and decay data used by MCB consist of:

- Decay data including decay constants and branching ratios for over 2400 nuclides. The decay data file was prepared on the basis of the Table of Isotopes (ToI) version 8E.
- Neutron transport cross section libraries for about 300 nuclides, prepared with NJOY at various temperatures on the basis of the room temperature evaluations ENDF/B-VI, JEF2.2 and JENDL3.2.

- Neutron reaction cross section libraries for about 400 additional nuclides (for which transport cross section evaluations do not exist), prepared with NJOY at various temperatures on the basis of the EAF evaluation.
- Continuous energy fission product yield libraries for 36 actinides, including yields of over 1000 fission products. The library was constructed using an updated version of the THERMO code, which calculates independent yields using a non-equilibrium thermodynamical model [2]. See below for details.
- Data for effective dose per unit intake for 738 nuclides, prepared on the basis of the Basic Safety Standards of IAEA.
- Meta-stable to ground state capture ratios for neutron capture on ^{241}Am and ^{243}Am according to the evaluation of Mann and Schenter [3].

All unique (with respect to nuclide) transport and reaction cross sections given in the XSDIR file are loaded during initialisation of MCB. Presently, it is the first occurrence of a nuclide that is loaded, if paths to different evaluations are given. During calculation, only cross sections for nuclides that have concentrations larger than a given threshold will be used. This threshold may be changed in the input file, which might have large influence on the time used by MCB for particle transport.

Material specifications

Material specifications are simplified with respect to the MCNP input format. In MCB, chemical symbols may be used instead of charge numbers, e.g. Pu239.60c replaces 94239.60c, and Pb replaces 82000.xxc. The evaluation index in the latter case is fixed by the first occuring library path in the XSDIR file. Specifying the index explicitly overrides the XSDIR file ordering.

In addition to standard MCNP material specifications “burnup”, “residual” and “mixed” materials are introduced in MCB. Burnup materials are not used in transport calculations unless their macroscopic cross section contribute to the total cross section with a fraction larger than a discrimination level supplied in the input file. Residual material have no defined density, and are used only for transmutation transition calculations. Finally materials may be mixed using the mixed material specification, which greatly simplifies initial system definitions.

Burnup run specifications

Materials for which burnup is to be calculated (not necessarily all materials) are specified with the “BURN” command. If several of the cells in the system geometry have the same material number, they will constitute a burnup zone, where nuclide evolution will be calculated from averaged transmutation rates. This can be used in symmetrical systems to diminish statistical fluctuations.

The physical conditions of the irradiation (and decay) simulation are fixed by specifying time periods of constant conditions, and corresponding source strength or heat dissipation (power). If neither power nor source strength is specified, or both are set to zero, plain decay of unstable nuclides takes place.

The constraints of the automated time-stepping routine are prescribed in the input file by specifying longest allowed time step (equal to the first trial time step), allowed variation of k-eigenvalue, neutron multiplication and/or reaction rate during a time step. Discrimination levels of macroscopic cross section contributions and nuclide to nuclide transmutation transitions may also be specified, as well as a half-life threshold for treatment of fast decaying nuclides. All these variables have default values, and hence are not required input data.

Flow sheet of code run

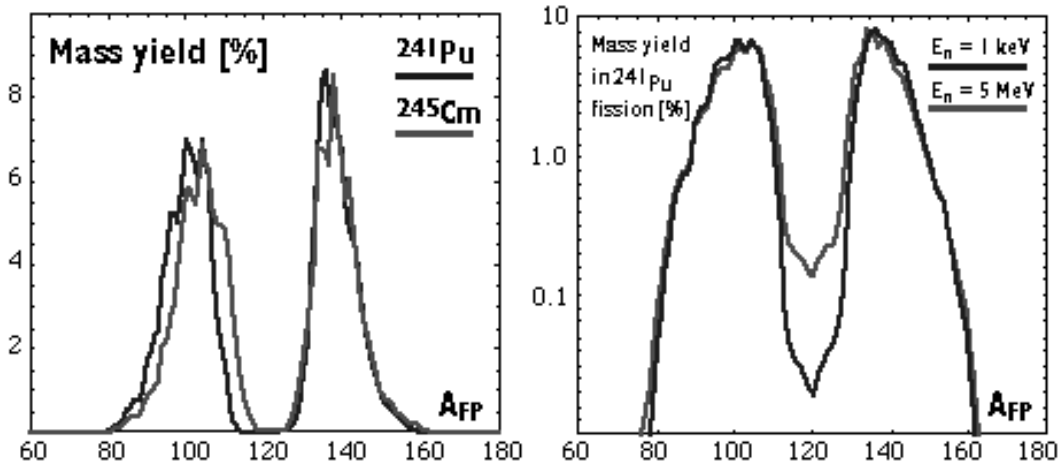
At start-up of the code, all unique cross section files pointed to in the XSDIR file are loaded, as described previously. The program checks if nuclides with short half-life exist in the materials specified, and force them to decay before making a calculation of the k-eigenvalue of the system. If this is lower than a given threshold, a source particle transport run is made where system power and transmutation rates are calculated "in flight". Otherwise, the particle flux is assumed to be sufficiently well described by the eigenflux and a new KCODE run is made, including sampling of heating and transmutation rates. Then, transmutation trajectories are selected, and the nuclide density evolution is calculated during the whole trial time step. The macroscopic cross sections of the appearing nuclides are calculated in order to check that they do not exceed the fraction of the total cross section set by the discrimination level. Similarly, a k-eigenvalue calculation is made to assure that changes in asymptotic neutron multiplication stays within the prescribed range. If either of these conditions are not fulfilled, a smaller time step is set for a renewed nuclide density prediction. Finally, new nuclide concentrations in the burnable materials are initialised and a new particle transport run is initiated.

Fission Product Yield Model

Since experimental data on fission product yields of the minor actinides are scarce, and the energy dependence of mass and charge distributions are only known for three points (at best), there was a need for a robust theoretical model to create energy dependent fission product yield libraries. In MCB, the non-equilibrium thermodynamical model of Grashin is used for this purpose [2]. The model is based on a new theoretical understanding of quantum mechanical processes in systems having too many free variables for non-statistical methods to be useful, while being too short-lived for standard equilibrium thermodynamics to be fully applicable. By introducing the concept of "free energy" of the excited compound nucleus, the model calculates the probability of finding final states of two (or three) fission products with concomitant release of a given number of neutrons within the manifold of the initial state. Thus the energy dependence of the fission product yield enters as a fundamental property in the model. Shell effects are taken into account , and most free parameters are fixed by fitting model predictions with experimental yields for a fission of a single nuclide at a single energy. For other nuclides only one free parameter, the ground state temperature, remains. This can be determined from e.g. the ratio of peak to fission valley yields, which is better known for the minor actinides than individual yields. Since yield distributions for thermal fission of ^{235}U are comparatively well known, errors in the low yield predictions for arbitrary actinides should generally not be worse than the same errors for ^{235}U. This is of great significance in transmutation simulations, as many system proposals are based on pure minor actinide fuels, which existing commercial codes never were intended to model accurately.

Figure 1 shows the predicted fission product mass yields at thermal incident neutron energies for ^{241}Pu and ^{245}Cm (left), and the energy dependence of the mass yield for ^{241}Pu (right).

Figure 1. **Fission product mass yields in thermal neutron induced fission of ^{241}Pu and ^{245}Cm (left). Incident neutron energy dependence of the mass yield in fission of ^{241}Pu (right). Note the differences in yield of the light peak and the fission valley, respectively.**



Note that the cumulative yield of ^{90}Sr varies considerably with mass of the fissioning actinide, being about 6% for ^{235}U, but less than 1% for ^{245}Cm. The increase of yield in the fission valley with neutron energy leads to an increased production of e.g. the raditoxic long lived nuclide ^{126}Sn by a factor of two when raising the incident neutron energy from 1 keV up to 1 MeV. The importance of including correct fission product yields in calculations of radiotoxic inventories thus seems very clear.

Discussion

The accurate modelling of high burnup waste transmutation systems demands a well validated integrated particle transport and burnup code. MCB, here presented, may fulfil this purpose. The main parts of the code being implemented and under testing, minor improvements still needs to be done before public release. The authors are well aware of the benefits of a large group of code evaluators, hence the release is expected to take place before the end of June 1999. Future versions of the code will include integration with MCNPX for high energy proton and neutron transport, as well as tallying of atomic recoil spectra for radiation damage estimations.

REFERENCES

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