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Original Article

DEVELOPMENT OF EASY-TO-USE INTERFACE FOR NUCLEAR TRANSMUTATION COMPUTING, VCINDER CODE

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A B S T R A C T

The CINDER code has about 60 years of development history, and is thus one of the world's best transmutation computing codes to date. Unfortunately, it is complex and cumbersome to use. Preparing auxiliary input files for activation computation from MCNPX output and executing them using Perl script (activation script) is the first difficulty, and separation of gamma source computing script (gamma script), which analyzes the spectra files produced by CINDER code and creates source definition format for MCNPX code, is the second difficulty. In addition, for highly nonlinear problems, multiple human interventions may increase the possibility of errors. Postprocessing such as making plots with large text outputs is also time consuming. One way to improve these limitations is to make a graphical user interface wrapper that includes all codes, such as MCNPX and CINDER, and all scripts with a visual C#.NET tool. The graphical user interface merges all the codes and provides easy postprocessing of graphics data and Microsoft office tools, such as Excel sheets, which make the CINDER code easy to use. This study describes the VCINDER code (with visual C#.NET) and gives a typical application example.

1. Introduction

Public radiation safety issues have long been one of the dominant concerns in human society. Recently, two big events, the North Korean nuclear bomb test and high magnitude earthquakes, have further alerted people to the issue of public safety, specifically, in regard to nuclear energy safety issues. Nuclear power plants harness the world's most concentrated energy source, but they have caused disastrous accidents, e.g., Three Mile Island, Chernobyl, and Fukushima [1]. Although average fatalities from nuclear accidents or terrorist attacks are not higher than those from alternative energy sources, long lasting serious radiological effects raise a higher public concern than any other energy source [2]. Thus, the importance of studying long lasting radiological effects cannot be overemphasized.

Radioactivity was discovered in 1896 by the French scientist Henri Becquerel while working with phosphorescent materials [3]. Ernest Rutherford was the first to realize that all such elements decay in accordance with the same mathematical exponential formula. Radioactivity is very frequently given as an example of exponential decay. The law describes the statistical behavior of a large number of nuclides, rather than individual atoms. Ernest Rutherford and his student Frederick Soddy were the first to realize that many decay processes resulted in the transmutation of one element to another. Thus, it is a sequence of radioactive decay processes: The decay of one element creates a new element that may itself be radioactive, which then continues to decay until the sequence ends with a stable nonradioactive atom.

The dangers of ionizing radiation due to radioactivity and x-rays were not immediately recognized and the biological effects of radiation due to radioactive substances were less easy to gauge. After World War II, the increased range and quantity of radioactive substances being handled because of military and civil nuclear programs led to large groups of workers and the public having the potential of being exposed to harmful levels of ionizing radiation, which led to the present International Commission on Radiological Protection [4]. Since then, the International Commission on Radiological Protection was definitely established as the leading international radiation protection authority and has published many reports that cover all aspects of radiation hazards. Thus, the evidence over six decades shows that nuclear power is a safe means of generating electricity. The risk of accidents in nuclear power plants is low and declining. The consequences of an accident or terrorist attack are minimal compared with other commonly accepted risks. Radiological effects on people of radioactive releases

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can be avoided owing to big achievements in understanding nuclear transmutation and transport physics phenomena.

As an activity to understand the exact nuclear transmutation in support of naval reactor design calculations, T. England at Bettis Atomic Power Laboratory developed a computer code (called CINDER) in the early 1960s [5,6]. The code solves the Bateman equation to estimate atom density (atoms per unit volume) and activity density (curies per unit volume) of all nuclides present at a specified time. The code is called a burnup code in nuclear reactor applications because it follows the temporal burnup of fissionable material and the associated production of fission products. It may also be called an activation code because it well describes activation—the conversion of stable nuclides to radioactive nuclides by particle collision. Practically, the code follows all possible paths of nuclide transmutation based on the CINDER library data—the conversion of a nuclide to a different nuclide by particle absorption and/or radioactive decay. Although significant improvements to both the CINDER code and underlying data library have been achieved [7,8], some stumbling blocks (e.g., human intervention between two Perl scripts for computing and analyzing activation or burnup problems) for easy use exist in view of the present advanced computing technology because of the long historical legacies involved in the code. The purpose of this study is to introduce an easy way (minimize the human intervention during computation and analysis) to use the code by providing a Microsoft Windows graphical user interface (GUI) in computing and analysis.

Microsoft Visual C# is Microsoft's implementation of the C# specification, which is included in the Microsoft Visual Studio suite of products [9]. It is based on the ECMA/ISO specification of the C# language created by Microsoft. Although there are many tools for realizing visual computing, Visual C# is by far the one most commonly used wrapper with the .NET framework tools [10]. In this study, we created a new VCINDER code using visual C#.NET, which provides a simple all-in-one interface to simulate nuclear transmutation phenomena. Implementation details are explained in the following section.

2. Materials and methods

2.1. Governing equation

A nuclide is a species of atom characterized by the atomic number (Z), mass number (A), and isomeric states (ground state, first isomer, second isomer, etc.). The nuclear isomers of interest are generally long-lived excited states, not short-lived excited states. Because statistical behavior of radioactivity decay is given by an exponential distribution, the differential equation describing the rate of change in the atom density $N_m(t)$, of a nuclide m is written as the sum of the rates of destruction and production in the nuclide density [11]:

$$dN_m(t)/dt = -N_m(t)\beta_m + \overline{Y}_m + \sum_{k \neq m} N_k(t)\gamma_{k\to m}, \quad (1)$$

where $\gamma_{k\to m}$ is the probability of nuclide k transforming (by absorption or decay) to nuclide m and β_m is the total transmutation probability of nuclide m defined by

$$\beta_m = \lambda^m + \phi\sigma_a^m \quad (2)$$

Here ϕ is the neutron flux calculated from energy integration, σ_a^m is the flux-weighted average cross section for neutron absorption by nuclide m, and λ^m is the total decay constant of nuclide m. Absorption reactions of σ_a^m are all of those with products other than nuclide m, and thus include only inelastic scattering to states other than that of nuclide m. $\overline{Y}_m$ is an additional constant corresponding to significant particle production (or depletion) because of neutrons with high energies above thresholds given to the CINDER library (>25 MeV) because the CINDER library includes only residual production cross-section data for neutron reactions below 25 MeV. The destruction rate is due to two mechanisms: (1) the radioactive decay of nuclide m producing daughter nuclides and (2) particle absorption reactions of nuclide m producing residual nuclides different from m. The production rate is the rate of other nuclides in the system that becomes nuclide m as a daughter or residual.

The drawback of applying governing equation (1) is that the transmutation probabilities β_m and $\gamma_{k\to m}$, and thus the flux ϕ are constant for the time interval for which the solution is desired. In the usual activation simulation code, any temporal history can be approximated using a histogram of constant-flux intervals. A few different solution methods are applicable: direct integration, matrix diagonalization, and reduction to a set of independent, linear differential equations using the Markov method that results in an analytical solution.

The first-order differential governing (Bateman) equation describing all nuclides is coupled because each nuclide atom density contains the sum over temporal atom density of all other nuclides. Thus, it is not exactly a linear chain. However, Bateman gave an analytical solution method by breaking it down into a set of linear chains, called the Markovian property, where the future is independent of the past if the current state is known. The CINDER code uses this algorithm, but the ORIGEN code uses a matrix calculus called the matrix exponential method, where the solution is obtained by truncating the power series for the exponential. It is clear that the applied series expansion has limited accuracy due to truncation and round-off errors. This study is concerned with the linearization method applied to the CINDER code.

2.2. Solution method

Coupled first-order differential equations are linearized using the Markovian property: the future is independent of the past if the current state is given. The time evolution of the nuclide concentrations is broken down into “chains” representing every possible reaction path. The solution is obtained by solving for the partial concentrations of each nuclide in a specific linear “chain,” including all possible chains and by summing these partial concentrations to obtain the total atom densities (Fig. 1) [12]. The Bateman equation

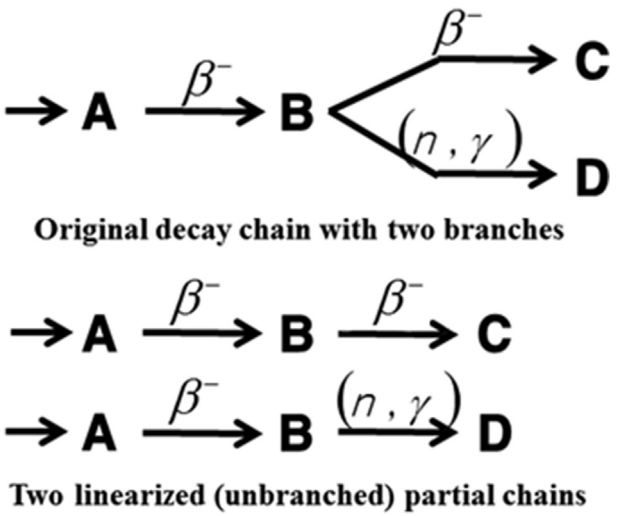

Fig. 1. Simple example of nuclide decay chain linearization.

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