COMPUTATIONAL FACETS OF RADIOACTIVE BOX (COMPARTMENT) MODELING

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Abstract

Wide applications of box modeling exist in radioactive decay, isotope production, nuclear engineering, astrophysics, health physics, chemical kinetics, biology, environmental and contaminant transport, *etc*. This presentation reviews the principles of box modeling and summarizes several years of experience with radioactive decay box modeling within the New York State Department of Health/SUNY nuclear chemistry program. The categories of box models in radioactive decay are described: sequential, branching, forward, reverse, and with non-equal or equal rate coefficients. There are nineteen reported computational methods to solve box models[1]; several of them are outlined in this presentation: by direct solution of differential equations, Laplace transform, matrix diagonalization, series expansion, Chebyshev polynomials, and Green's function. For forward branching box model, an efficient recursive algorithm is presented in Fortran 90 for calculation of the radioactive decay matrices. Incorporation of events such as chemical separation into radioactive box modeling is described. Examples of application of box models to uranium natural decay series[2] and to isobaric A = 90 and A = 137 fission-product yields[3] are given. Possible methods of uncertainty propagation for the box modeling are presented.

1. C. Moler, C. Van Loan. Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. *SIAM Review* **45** (2003) 3-49.
2. T.M. Semkow, P.P Parekh, C.D. Schwenker, R. Dansereau, J.S. Webber. Efficiency of the Lucas scintillation cell. *Nucl. Instr. Meth. Phys. Res. A* **353** (1994) 515-518.
3. T.M. Semkow, P.P. Parekh, D.K. Haines. Modeling the effects of the Trinity test. In: *Applied Modeling and Computations in Nuclear Science*, ACS Symposium Series **945**, Oxford University Press (2007) 142-159.