X.M. SAMSMC: MONTE CARLO MULTIPLE SCATTERING

In Section III.D, SAMMY's method of calculating the multiple-scattering corrections to the capture and fission yields is presented. Because these calculations involve complicated expressions as well as approximations whose legitimacy can be questioned, it is desirable to have an independent means of testing the calculations. Monte Carlo is suitable for this task, as the method is completely different from the analytic-with-approximations approach taken in Section III.D.

The precursor to the code SAMSMC was written during the 1980's by Gerard de Saussure [GD80] and subsequently modified by Francis Perey. More recently, the SAMMY author has modified this code to include anisotropic scattering (non-s-waves) and more than one nuclide. In addition, an interface was developed with the SAMMY code, in order for SAMSMC to read and use the same Doppler-broadened cross sections and energies that are used in SAMMY.

Use of the SAMSMC code is a multi-step process, described below.

1. Run SAMMY with a line in the alphanumeric section of the INPut file which says

   ```
   PREPARE INPUT FOR MONte carlo simulation
   ```

   This command causes the code to stop at the point where it would otherwise begin execution of segment SAMSSM. Two or three files are produced that are needed for the Monte Carlo simulation: File SAM54.DAT contains the unbroadened cross sections and SAM51.DAT contains Doppler-broadened cross sections (assuming the INPut file specified that Doppler broadening was to be done). Rename these file for use in later steps.

   The third file is SAMMY.MCR, which contains most of the information to be given to SAMSMC (as specified in # 2 below). Some of this information you will use as is; other values may be modified.

2. Run program SAMSMC (SAM-Ssm-Monte-Carlo), with the following lines of input:
   a. Title (whatever you wish)
   b. Energy-mesh information (Emin, Emax, 0.)
   c. Name of file with energy mesh (here only if Emin = 0 in part a)
   d. THSAMP, XSAMP, YSAMP, XBEAM, YBEAM (like card set 11 in INPut file for the regular SAMMY run)
   e. Thickness (in atoms/barn), Mass (in amu)
   f. Maximum number of histories
   g. Number of scatterings to include
   h. Name of the file generated by SAMMY run of step 1 (renamed from SAM51.DAT)
   i. Maximum *L*-value in that file (where *L* is the vector sum of the orbital angular momentum for the individual levels); number of nuclides
   j. Normalize as yield (Y) or cross section (C) or other (O)
   k. If more than one nuclide, give masses of each
   l. If more than one nuclide, give abundance for each

Two output files are produced by the SAMSMC run. MC_1.DAT holds the various cross sections, and MC_2.DAT contains results from 0 scattering, 1 scattering, two-or-more scatterings, and the sum of those three. Rename these, if desired.

3. Run program SAMSMX (SAMSMc-fiX), with the following input:
   a. Name of the cross section file produced by SAMSMC (MC_1.DAT)
   b. Name of the second file produced by SAMSMC (MC_2.DAT)

   Four output files are produced by this run. Three are ASCII files name MC_Y0.DAT, MC_Y1.DAT, and MC_Y2.DAT; these contain the self-shielded yield, the self-shielded plus single-scattering-corrected yield, and the full multiple-scattering-corrected yield, respectively. These files are in a form suitable for use as SAMMY DATa files, in the TWENTY format (see Section VI.C.1).

   The other output file produced by this procedure is named MC.ODF. This file is an ODF file (see Section VII.C) with the following sections:

   S1. energy in eV
   S2. 0 scattering (self-shielding) only
   S3. 1 scattering
   S4. 2 scatterings
   S5. 0 + 1
   S6. 0 + 1 + 2
   S7. capture cross section
   S8. total cross section
   S9. (1-exp(-thickness $\times$ total cross section)) $\times$ capture / total

   Sections of this file can be compared to output in section 4 of the ODF file produced by the corresponding SAMMY runs. For example, output from a SAMMY run that includes single scattering (finite disk) but not double scattering would be compared to Section 5 in MC.ODF.