

III. CORRECTIONS FOR EXPERIMENTAL CONDITIONS

In general it is not possible to directly compare the cross sections extracted from experiments to those generated via R-matrix theory (or via any other theory). This is because “perfect” experimental conditions do not exist: (1) individual nuclei within the sample are not at rest; (2) finite time intervals are required both for the neutron beam and for the detecting apparatus; (3) the flight-path length traversed by a neutron depends on its position of origin within the neutron-producing target, on its position of interaction within the sample, and on the position at which it is detected; (4) the finite size of the sample causes interactions beyond those described by the cross section for individual nuclei. The first of these conditions leads to the effect known as Doppler broadening, the second and third lead to resolution broadening, and the fourth to multiple-scattering and self-shielding effects. There are other effects as well, not included in this enumeration. To compare theory to experiment, either the theory must include these effects or corrections must be applied to the experimental data. Often the former is easier, or the latter is impossible. SAMMY therefore includes options to simulate a great many of these effects, and modify the theoretical calculations appropriately.

To simulate Doppler or resolution broadening (i.e., to “broaden the theory”), it is necessary to first have a mathematical description of the broadening (generally, as an integral of the unbroadened cross section times a broadening function), and then to evaluate those integrals analytically if possible or numerically if necessary.

In Section III.A, the scheme used in SAMMY for most of the numerical integrations is described in some detail. It is important to note that it is the *user*, not the code author, who is responsible for ensuring that the numerical integrations are performed sufficiently well; this is discussed in Section III.A.1, which should be read and carefully considered before analysis results are published.

SAMMY contains four distinct procedures for Doppler broadening, which are described in Section III.B. The various available methodologies for resolution broadening are discussed in Section III.C. Section III.D is devoted to multiple-scattering effects, and other phenomena are treated in Section III.E.