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The state of the art of GENFIT, an advanced software for the analysis of SAS data

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GENFIT is a well-established software tool for analysing small-angle scattering (SAS) data from X-ray (SAXS) or neutron (SANS) experiments. It reads a set of one-dimensional scattering curves and fits them using different kinds of models [1-8]. SAS curves calculated from a model can be smeared to allow for the instrumental resolution. The user can fit the experimental data selecting one or more models from a list including, to date, more than 90 models, starting from simple asymptotic behaviours down to complete atomic structures. Some models are defined in terms of both form and structure factors. GENFIT is able to simultaneously fit more SAS curves via a unique model or a mixture of models. In the latter case, some specific model parameters can be shared by any selection of the experimental curves. Model parameters can be related to the experimental chemical-physical conditions (temperature, pressure, concentration, pH, etc.) as well as to thermodynamic or kinetic models by means of link functions, which can be freely defined by the user. The main features of GENFIT and a few examples of its use will be presented, together with some indications of possible future developments.

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