EMPIRE optional input keywords

The optional input allows modifications to the default model parameters. Optional input consists of an arbitrary number of records, entered in any order and closed with the GO record, which indicates the end of the input. In the simplest case (all defaults), only the GO record must be entered.

Each optional record starts with an alphanumeric keyword **NAME**. If the first character of the line (i.e. **NAME(1:1)**) is *, # or **!**, then this line contains comments and is ignored by the code. There might be an arbitrary number of comments line in the optional input. If the first character of the line **NAME(1:1)** is **@**, then this line contains a title, which will be printed in EMPIRE outputs; obviously the title is not used in any calculations. Multiple titles are allowed. Users are strongly encouraged to use titles and comments in EMPIRE inputs; that will be a significant step toward a better documentation of our theoretical calculations and evaluations.

The optional-input keyword **NAME** is followed by the value VAL and four positional parameters I1, I2, I3, I4. The keyword indicates a physical quantity, such as the binding energy or level density parameter or scaling parameter. VAL takes the numerical value of the given quantity or scaling parameter.
The positional parameters are typically used to specify to which nucleus the quantity should be applied (generally if these are omitted the value is applied to all nuclei in the given calculation). Positional parameters may be also used to indicate the estimated uncertainty of the quantity defined by the input keyword (except optical model parameters for which the uncertainty is defined by VAL). Each record must be in the FORTRAN format:

FORMAT (A6,G10.5,4I5) **NAME**,VAL,I1,I2,I3,I4

Fixed format allows to avoid typing zeros if no input is needed for some positional

parameters.

The GO record indicates end of the optional input and starts calculations. It may be followed by an unlimited list of incident energies (and titles or comments) (one per record) terminated with a record containing a negative value. Anything below this line will be ignored by the code.

Calculation control

NEX Maximum number of energy steps in the integration set to VAL (default: min(50, NDEX)). NDEX parameter is defined in the *dimension.h* file.

ENDF Controls output for ENDF formatting and exclusive/inclusive emission

= 0 no ENDF formatting (default).

> 0 output for the full ENDF formatting will be created (including double differential MF=6) as shown in the two examples below

= 2 means all reactions emitting 2 or less particles are exclusive the rest are inclusive (lumped into MT=5)

= 3 means all reactions emitting 3 or less particles are exclusive the rest are inclusive (lumped into MT=5)

RECOIL Controls calculation of recoils,

= 0 recoils are not calculated (default if ENDF = 0, no ENDF formatting)

= 1 recoils are calculated (default if ENDF > 0, ENDF formatting)

If keyword ENDF=0 is given in the input, then recoils are not calculated independently of the keyword RECOIL.

PRGAMM Controls calculation of primary gammas

= 0 Primary gammas are not printed (default)

> 1 Primary gammas are printed

If keyword ENDF=0 is given in the input, then primary gammas are not printed independently of the keyword PRGAMM.

HRTW Controls HRTW calculations (width fluctuation correction)

= 0 no HRTW

> 0 HRTW width fluctuation correction up to the energy set by VAL.

FISSPE Controls calculation of prompt fission neutron spectra (PFNS).

= 0 PFNS are not calculated (default)

= 1 PFNS are calculated using Los Alamos model [**?**]

= 2 PFNS are calculated using Kornilov parameterization [**?**]

BENCHM Controls if benchmark calculation is requested.

= 0 no benchmark calculation (default),

> 0 benchmark calculation requested. Energies do not need to be in increasing order.

KALMAN Controls calculation of a sensitivity matrix,

= 0 no sensitivity matrix calculations (default),

= 1 sensitivity matrix is calculated.

RANDOM Controls randomization of input parameters that were input with uncertainty

= 0 no random sampling is allowed (default)

> 0 random sampling based on normal (Gaussian) distribution with the given 1-sigma parameter uncertainty

< 0 random sampling based on uniform distribution with the given 1-sigma parameter uncertainty

ISOMER The minimum isomer half life (in seconds) set to VAL

This keyword defines minimum half-life of the state to be considered an isomer (default 1. = 1 second)

Output control

IOUT Main output control set to VAL

= 1 input data and essential results (all cross sections) (default),

= 2 as IOUT=1 plus fusion spin distribution, yrast state population, γ-transition parameters, fusion barrier, inclusive spectra,

= 3 as IOUT=2 + γ and particle spectra + discrete levels' decay + double differential cross sections (if MSD>0),

= 4 as IOUT=2 + ORION output + residual nuclei continuum population (up to spin 12),

= 5 as IOUT=2 + ORION output + transmission coefficients (up to l=12),

= 6 as IOUT=2 + ORION output + level densities (up to spin 12). Should be used to get ZVV level density plots.

NOUT MSC calculation output control set to VAL (default: 0).

Optical Model Potential

OMPOT Selects optical model parameters for outgoing particle

The value of I1 selects the outgoing particle as follows:

=1 neutrons,

=2 protons,

=3 alphas,

=4 deuterons,

=5 tritons,

=6 He-3;

VAL must be set to a RIPL catalog number (e.g. 2408 for Capote et al OMP) of the potential as it appears in the empire/RIPL/optical/om-data/om-index.txt file or in Help => 'RIPL omp' when using GUI. For backward compatibility this number can be entered with a negative sign.

DIRPOT Optical model parameters to be used in DWBA or coupled-channels calculations by ECIS/OPTMAN codes. Parameters are the same as above, except that I1 need not be specified (always refers to the incident channel).

RELKIN Override the RIPL defined kinematics used in a given optical model potential,

= 0 classical (default),

= 1 relativistic.

TRGLEV Excited level of the target is set to VAL (e.g., VAL=3 for the 2^{nd} excited state; default: 1 (ground state)).

UOMPab Uncertainty of the parameters defining the potential strength of the optical model potential. The letter a can be V (real potential strength) or W (imaginary potential strength). The letter b can be V (volume) or S(surface). Thus the combinations VV (real volume), WV (imaginary volume), and WS (imaginary surface) specify 3 different terms in the RIPL optical potential described in Section **??**. The combination VS is not allowed, as parameters of the real surface potential (VS) are usually not used in deriving phenomenological potentials. The exception is for dispersive potentials, but in this case the VS uncertainty is fully determined by the uncertainty of the imaginary surface potential (WS). The uncertainty of the spin-orbit potential is also not considered as its influence on calculated cross sections is small.

The relative uncertainty in % of the corresponding parameter (defined by letters a and b) is given by VAL, target's Z and A numbers

are defined by I1 and I2, respectively. I3 defines the outgoing particle, i.e., the incident particle for the inverse reaction (I3=1 for neutron, I3=2 for protons, etc).
Some examples of potential strength uncertainties are given below.

```
* The three lines below define 1.5% uncertainty of the real
* volume potential strength and 10% uncertainty of the real
* and imaginary surface potential strength for neutron and
* proton emission channels from the 56-Mn compound nucleus
UOMPVV   1.50000  25    55   1
UOMPWV  10.0000   25    55   1
UOMPWS  10.0000   25    55   1
* The same for the proton emission channel
UOMPVV   1.50000  24    55   2
UOMPWV   2.5000   24    55   2
UOMPWS  10.0000   24    55   2
```

UOMPcd Defines the uncertainty of the geometry component of the optical model potential. The letter c can be R (radius) or A (diffuseness). The letter d can be V (real volume), W (imaginary volume) or S (imaginary surface). Thus the following six combinations are possible: RV and AV (real volume radius and diffuseness), RW and AW (imaginary volume radius and diffuseness), and RS and AS (surface radius and diffuseness).
The relative uncertainty of the corresponding parameter (defined by letters c and d) is given by VAL (in percent), target's Z and A are defined by I1 and I2, respectively. I3 defines the outgoing particle, i.e. the incident particle for the inverse reaction (I3=1 for neutron, I3=2 for protons, etc).
It is recommended to avoid variations of potential strength (e.g. VV,WV) and corresponding potential radius (e.g. RV, RW) in the same run, as those parameters are strongly correlated within the optical model.
Some examples of geometry uncertainties of the optical model parameters are given below.

```
* The two lines below define 1.5% uncertainty of the
* imaginary volume radius, and 2.5% uncertainty of the
* imaginary volume diffuseness for a neutrons incident
* on 55Mn nucleus
UOMPRW   1.50000  25    55   1
UOMPAW   2.5000   25    55   1
* The same for the proton emission channel
```

```
* corresponding to the surface potential.
UOMPRS   1.50000  24    55   2
UOMPAS   2.5000   24    55   2
```

Scattering on collective levels

EMPIRE includes two coupled-channels codes: ECIS and OPTMAN[**?**]. ECIS is the default optical model solver, but OPTMAN should be used for selected potentials, when soft-rotor couplings are desired, as well as for actinide potentials that couple levels beyond the ground state rotational band.

DIRECT Controls use of coupled-channel calculations (ECIS and OPTMAN)

- **=0** spherical OM used (default)
- **=1** Coupled Channel (CC) method used for calculation of inelastic scattering to collective levels in the incident channel. If a selected OM potential is of CC type, the elastic and reaction cross sections are also taken from ECIS/OPTMAN calculations. Otherwise, spherical OM results are used. Transmission coefficients for all outgoing channels are calculated with spherical OM.
- **=2** as above but transmission coefficients for the inelastic outgoing channels are calculated within Coupled Channel approach (longer calculation time).
- **=3** as DIRECT=1 but DWBA is used instead of CC for calculation of inelastic scattering to collective levels in the incident channel. All transmission coefficients calculated with spherical OM.

NOTE: OM potential to be used by ECIS/OPTMAN might be different from the one used in the rest of the calculations and can be specified with the DIRPOT option.

CALCTL Controls use of calculated transmission coefficients for both projectile and ejectiles.

= 0 Transmission coefficients calculated during the first run are stored, and reused in subsequent EMPIRE runs (default),

> 0 Transmission coefficients are calculated independently for each run; no reusage is allowed. This option is useful to calculate some quantities that are only used if TL are not already present (e.g. Bass fusion barrier in HI induced reactions). However, this potion slows down the execution of the code in subsequent runs up to a factor of

10 times (additional time is needed to calculate TLs again; reading them is much faster.

EcDWBA Automatically selects all discrete levels to be used in DWBA calculations for uncoupled collective levels.
The default cut-off energy is $3 * 30/A^{2/3}$, and the default maximum spin 4. With these defaults all levels ($J < 5$) with excitation energy less than 2.4 MeV for ^{238}U), and less than 6.2 MeV for ^{56}Fe are considered.
The default selection rules could be modified by the VAL parameter that redefines the cut-off energy, and the parameter I1 that sets the maximum spin.

RESOLF Energy resolution in MeV used to spread calculated collective cross sections in the continuum set to VAL.
This parameter is used if there are collective levels (in the *-lev.col file) that are located in the continuum (see the *cont* flag). The scattering cross sections on these levels will be calculated by DWBA (if keyword DIRECT > 0).

DEFNUC Deformation of the target nucleus set to VAL.
The threshold value to assume that the nucleus is deformed is 0.1 If you want to force the assumption of sphericity for a given nucleus you can use this parameter with a value less than 0.1 this parameter also affects the deformation used in MSD calculations.

Scaling parameters correcting for model deficiencies

These parameters are non-physical parameters designed to be used in nuclear data evaluation to correct for reaction model deficiencies, and to define model parameters' uncertainties. They are also used for covariance calculations by providing a straightforward way to calculate sensitivities (required as input for KALMAN), and to allow for random sampling of model parameters within defined uncertainties (required for Monte Carlo generation of theoretical model covariances).

TUNE The equilibrium decay width Γ_i^{EQ} of the ejectile i given by I3, for the nucleus with Z=I1 and A=I2 will be multiplied by VAL.
Estimated relative uncertainty in % of this parameter can be given by I4.

TUNEFI The fission decay width Γ_F will be multiplied by VAL for the nucleus with Z=I1 and A=I2.
Estimated uncertainty of this parameter can be given by I3.

TUNEPE The preequilibrium decay width Γ_i of the ejectile i given by I1 will be multiplied by VAL. It applies only to the PE decay from the compound nucleus calculated by PCROSS (exciton model), input keyword PCROSS > 0.
Estimated relative uncertainty in % of this parameter can be given by I2.

PFNNIU Used in prompt fission neutron (PFN) calculations. The evaluated total prompt neutron multiplicity $\widetilde{\nu}$ (read from NUBAR-EVAL.ENDF) will be multiplied by VAL (default: 1.). The relative uncertainty of the scaling factor in % could be given by I1.

PFNTKE Used in prompt fission neutron (PFN) calculations. The total kinetic energy (TKE) of the fission fragments will be multiplied by VAL (default: 1.). The TKE enters the energy balance equation defining the total excitation energy of the fissioning system $U_{exc} = E_{rel} - TKE + E_{incid} + B_n$. This parameter could be interpreted as the uncertainty of the measured fission kinetic energy.
The relative uncertainty of the scaling factor in % could be given by I1.

PFNALP Used in prompt fission neutron (PFN) calculations. The default parameter α ($\alpha_0 = 1$ for Madland-Nix (LA) model and α_0 0.9 for Kornilov parameterization) will be multiplied by VAL (default: 1.). The values E_f^L and E_f^H of the average kinetic energy per nucleon of the average light fragment AL and average heavy fragment AH are scaled by α. The effect of this parameter on PFNS calculations will be corerelated with TKE (see keyword PFNTKE above). // Physically, this parameter allows for a reduction of the kinetic energy of the fragment due to neutron emission during Coulomb acceleration.
The relative uncertainty of the scaling factor in % could be given by I1.

PFNRAT Used in prompt fission neutron (PFN) calculations. The default parameter $r = T_f^L/T_f^H$ ($r_0 = 1$ for Madland-Nix (LA) model and $r_0 = 1.248$ for Kornilov parameterization) will be multiplied by VAL (default: 1.). This parameter defines the ratio of temperatures of the light to heavy fragment. Recent evidence strongly supports 20% higher temperature of the light fragment.
The relative uncertainty of the scaling factor in % could be given by I1.

PFNERE Used in prompt fission neutron (PFN) calculations. The total fission