

Instructions for NON-SMOKER(web) v5.8w

Dr. Thomas Rauscher

Table of Contents

<u>Details and Instructions for NON-SMOKERWEB Version 5.8w</u>	1
<u>1. Explanation</u>	1
<u>General</u>	1
<u>Registration</u>	2
<u>Running NON-SMOKERweb</u>	2
<u>Custom input file</u>	3
<u>Applicability of the model</u>	6
<u>Referencing the results</u>	7
<u>Error messages</u>	7
<u>Bug reports</u>	7
<u>2. History</u>	7
<u>24-Aug-2006</u>	7
<u>20-Aug-2006</u>	7
<u>01-Jun-2006 to 02-Jun-2006</u>	7
<u>01-Apr-2006</u>	8
<u>09-Jul-2005 to 11-Jul-2005</u>	8
<u>15-Mar-2005</u>	8
<u>1-Mar-2005</u>	8
<u>25-Feb-2005</u>	8
<u>24-Feb-2005</u>	8
<u>21-Feb-2005</u>	8
<u>25-Oct-2004</u>	8
<u>7-Oct-2004</u>	8
<u>22-Sep-2004</u>	8
<u>Advanced Instructions for NON-SMOKERWEB v5.8w</u>	9
<u>Custom input file</u>	9
<u>Advanced options</u>	9

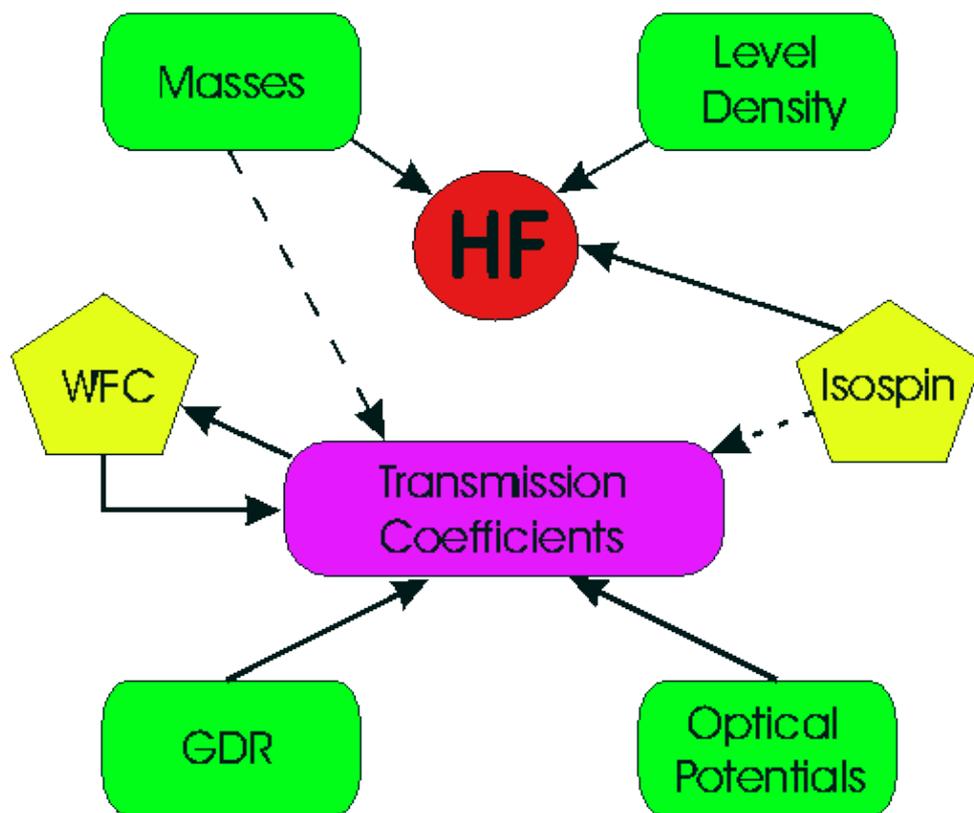
Details and Instructions for NON-SMOKER^{WEB} Version 5.8w

1. Explanation

General

NON-SMOKER^{WEB} is a Hauser-Feshbach statistical model code optimized for an energy and temperature range which is interesting for astrophysical purposes. It is related to the well-known SMOKER and NON-SMOKER codes.

Calculations in the statistical model require the input of a number of different nuclear properties:



Although the model is well-established, different calculations vary in the various inputs and treatments of such properties. In the calculations presented here, it was attempted to find descriptions which can be used to predict nuclear properties also for nuclei far off stability for which no experimental data is known. Therefore, it was tried to minimize the direct input of experimental data (although some parametrizations are fit to available nuclear data). Thus, we are interested in descriptions which lead to a low *average* deviation between predicted and observed properties. Nevertheless, local deviations of higher magnitude can occur.

Instructions for NON-SMOKER(web) v5.8w

Different options can be chosen as input to the statistical model calculation. The default values are those used in the calculations published in [ADNDT 75 \(2000\) 1](#) and [79 \(2001\) 47](#) (except for experimental masses which have been updated since). For a more detailed explanation of the options see those papers and the [reference section](#).

Important note: The default settings of the code make use of *global* inputs, attempting to include as few local information as possible. For a fair comparison to other codes be aware that many other codes include a lot of local information (such as level densities or GDR properties) for nuclei at stability. When performing such comparisons, the NON-SMOKER^{WEB} settings should be chosen accordingly!

Registration

To run NON-SMOKER^{web} the user has to be registered. If you want to start a collaboration and use NON-SMOKER^{web} please use the [Registration Form](#), specifying in detail what you want to use the code for. You will then be sent a username and password shortly. The access may be restricted to certain targets or projectiles and certain options.

Running NON-SMOKER^{web}

The [HTML interface](#) should be quite self-explanatory. In the element box, the standard abbreviation of the element should be input, as it is used in periodic systems or nuclear charts; e.g. Ne for Neon or au for Gold (input is not case sensitive). The massnumber is an integer with 2 or 3 digits.

Options and Output

The recommended set of options is the default, therefore it should be sufficient in most cases to just enter element and mass number and to select which kind of projectile one wants to use. The output will contain the nuclear reaction cross sections for three different channels (gamma, n, p, alpha) depending on which projectile was chosen. It will also contain the astrophysical reaction rates. For reactions with a neutral projectile, the Maxwellian averaged cross sections (MACS) are additionally written whereas for charged particle induced reactions the astrophysical S-factor is additionally written. For astrophysical applications it is not only necessary to know the reactions on targets in the ground state but also on thermally excited targets. The reaction rates and MACS are both given for g.s. and thermally excited targets, cross sections and S-factors only for targets being in the g.s.

Theoretical masses: By default, in the calculations experimental values are used if available (for the current status of the experimental masses included, see also the [history section](#)). The setting of the theoretical mass will affect experimentally unknown masses (separation energies), as well as the level density for *all* nuclei if the default level density is chosen.

The FRDM covers the widest mass range, ETFSI values are available only for $A > 35$, and the ETFSIQ table starts at Cr ($Z > 23$).

Hint: The output can be saved by right-clicking *into* the returned page and then selecting "Save as..." and the appropriate format (usually, that is text format). This yields a nice text file which can be inspected further. (For further hints, [see below](#).)

Custom input file

Using a custom input file offers even more flexibility than the options directly provided on the [web page](#). In order to use a file, the appropriate option on the [web page](#) has to be checked and a file location has to be provided in the appropriate field. On submission of the [web form](#), the file will be loaded and the appropriate data used (if the file contains more than the data required by the checked options, the excess data will be ignored). For each calculation, the input file will be loaded again from the specified location. The input file is an ASCII file which contains options and data in a [specific format](#). Invalid input files will trigger error messages.

Input file format:

- Basics:
 - ◆ The input file is a plain ASCII file (text file). The name of the file is irrelevant but some browsers do not assume to be sending a plain text file when the extension is something else than `.txt`, `.dat`, or `.inp` and they might encode it inappropriately. Therefore one of these file extensions should be used preferentially. Take a look at the [sample input file](#) (the data contained therein is just for illustrative purposes and does not have any real physical meaning) and modify it for your own purposes.
 - ◆ The maximum length of a line in the input file is 500 characters. If that length is exceeded, errors or unwanted behavior of the code may result!
 - ◆ Data is organized into sections which start with an identifier and end with the general end-identifier `END`. The order of the sections is irrelevant but they have to be between the `INPUT_START` and `INPUT_END` labels. Everything outside of these labels or between sections is ignored.
 - ◆ `NON-SMOKERweb` uses input only from sections which correspond to the options selected on the [web form](#). All other data is ignored.
 - ◆ Section labels (identifiers) and special labels start with `'#*'`. They are case sensitive!
 - ◆ Comment lines use an `'#'` as first character (and don't have an `'*'` as second character) and can appear everywhere. Blank lines are ignored.
- Some details:
 - ◆ Optical potentials:
 - ◇ Section labels: `CUSTOM_ALPHA`, `CUSTOM_NEUTRON`, `CUSTOM_PROTON`.
 - ◇ For the proton and alpha potentials, the first entry in the section defines the Coulomb radius r_c . The value of the radius has to follow the label on the same line:
`#*RCOUL 1.2`
 (For the neutron potential there is no such line; it is an error if such a line is present.)
 - ◇ Within these sections there are two subsections each (both have to be specified): The real part of the optical potential is defined from the beginning of the section to the label `REALEND`; the imaginary part is defined after the label `REALEND` up to the `END` identifier.
 - ◇ Within each of the two subsections, there are two ways to specify the potential: Either by explicitly giving data points or by providing an algebraic expression to compute the potential. The first method is selected with the label `DATA`, the second with `EXPRESSION`. Each of these labels have to be given before any data or expression in that subsection.
 - ◇ *Option DATA*: Pairs of radius (in fm) and potential depth (in MeV) are given. At most 800 pairs can be given. They don't have to be equidistant but have to be in ascending order by radius (and all radii have to be different). Points between the given data are linearly interpolated. At least two pairs have to be given explicitly. Above and below the first and last point, respectively, the potential is extrapolated using the same slope

Instructions for NON-SMOKER(web) v5.8w

as between the last two known points. (If you want the potential to become constant, specify a depth twice.)

◇ *Option EXPRESSION*: Specify a function to compute the optical potential part at a given radius. See the [detailed explanation of custom potentials](#) below. Any whitespace characters (including blanks, tabs, newlines) are ignored, they can be used to structure the input for better (user) legibility. The current upper length limit is 500 characters (not counting whitespace).

◆ Level density:

◇ Section label: `CUSTOM_LEVEL_DENSITY`

◇ Custom parameters for a shifted Fermi-gas description of the nuclear level density can be provided here. The order of parameters is charge Z , mass number A , level density parameter a (in MeV^{-1}), shift Δ (in MeV).

◇ During a calculation the default level density (see [web page](#)) is used unless Fermi-gas parameters have been specified for that nucleus. In the latter case a Fermi-gas level density with those parameters is used. At low excitation energies, a constant temperature formula is used in both cases to avoid the divergence of the Fermi-gas description.

◆ Masses

◇ Section label: `MASSES`

◇ Each entry contains charge Z , mass number A , and the mass excess (in MeV).

◇ During a calculation the default mass (either experimental or theoretical, see [web page](#)) is used unless the mass excess for that nucleus has been specified in the input file. An explicitly defined mass excess is always used when it is found in the input file.

◇ To change a separation energy, specify the proper two masses but keep in mind that an altered mass also may affect the separation energies in other reaction channels.

◆ Excited states:

◇ Section label: `EXCITED_STATES`

◇ Low-lying excited states can be specified for a number of nuclei. Each nucleus has its own subsection which starts with the specification of charge Z and mass number A , and ends with the label `NUCEND` (or `END` for the last nucleus in the list).

◇ After the Z - A identification of the nucleus, a list of nuclear states follows with one entry per line, giving excitation energy (in MeV), spin (in multiples of $1/2$), and parity (positive/even parity when the spin integer is \geq zero, negative/odd parity with spin $<$ zero).

◇ The ground state (zero excitation energy) has to be included!

◇ There is an upper limit of how many states (including g.s.) can be specified. This depends on the code version you are using. More states will not trigger an error message but will simply be ignored.

◇ If no states are explicitly specified for a given nucleus, the default states (from Table of Isotopes) are used. Otherwise, the default levels are superseded by the ones in the input file.

◇ *Breit-Wigner Resonances*: `NON-SMOKERweb` can also calculate Breit-Wigner resonance parameters and cross sections.

· For the compound nucleus of the reaction, put in excited states *above* the separation energy of the projectile (this only works for neutron- and proton-induced reactions). This will prompt `NON-SMOKERweb` to also compute and output the Breit-Wigner data.

· Most likely the other output (cross sections, rates, ...) is meaningless in this case. Remember that there still is a limit on the number of states including the g.s. (see above). Try to put in as many low-lying resonances as possible,

though.

- ◆ Target range:
 - ◇ Section label: TARGET_RANGE
 - ◇ There are two ways to specify more than one target. These are distinguished by the labels EXPLICIT and GRID, respectively, which have to appear before any data in this section. If the label EXPLICIT is found, a list of target nuclei is expected to follow, one per line. With the option GRID, a range can be defined.
 - ◇ Option EXPLICIT: Specify charge Z and mass number A of a target nucleus. There can be several lines like that, each specifying another target nucleus.
 - ◇ Option GRID: Specification of a Z-N range of target nuclei. The order of supplied values is Z_start N_start Z_end N_end. There can only be one line of this kind.
 - ◇ Options EXPLICIT and GRID cannot be mixed.
- Some hints:
 - ◆ Before submitting an input file, check its validity with the **checker tool**! This is a C program which accepts a file name on the command line and returns more detailed error messages than the web interface (which will only tell you that there was a problem with the file). You need a C-compiler to make an executable for your architecture. Precompiled executables are provided for Linux and DEC Alpha.
 - ◆ It is advisable to keep a log on what you have changed in the input file during different runs. The result page returned by NON-SMOKER^{web} only shows the selected options but not the content of the file, unless the "Echo file content" checkbox is selected. Even in the latter case, the whole input file is echoed, not just the selected sections.
 - ◆ Since only those sections are used which have been selected in the options, sections in the input file can be selectively switched on and off without the need to remove or modify them.
 - ◆ On the other hand, if you want to make changes in the input file but not in the selected options, you can just hit the reload/update button on your browser to start a new calculation.
 - ◆ Access control restrictions apply equally to the options on the web page and to the input file. It is not possible to select sections in an input file for which the user does not have access permission.
 - ◆ For expert users, there are also advanced options available. Do not bother with those unless you really know what you are doing!

Custom potential:

A speciality in this interface is the possibility to put in new functions for the optical potentials. If you are not satisfied with the provided options, you can provide a potential in the custom area. Here are some guidelines what to put into the fields:

- Functions can be written as FORTRAN style expressions, including brackets. The input is not case sensitive.
- Whitespaces (blanks, tabs, newlines) are ignored in the evaluation of the expression. This can be used to more nicely structure the input. Note that the allowed line length in the input file may be shorter than the maximum length of the expression! For a longer expression it is strongly suggested to distribute it across several lines. Otherwise an error may result.
- The standard arithmetic operators + - * / are known. Exponentiation can be written either as ** or as ^. Additionally, the following functions are known:
 - ◆ exp(x)...exponentiation of Euler's number, e^x
 - ◆ log(x)...natural logarithm of x
 - ◆ sqrt(x)...Square root of x

The usual limits on the arguments of those functions apply.

Instructions for NON-SMOKER(web) v5.8w

- For comparison of two values, the test operator '<' can be used. (Note that there is NO '>' operator!) An expression $x < y$ will return 1 if x is smaller than y and 0 otherwise. This can be used to switch between different potential behavior depending, e.g., on the energy. See the examples below on how to use the operator. The operator precedence is stronger than $+ - * /$ but equal to exponentiation and the functions \exp , \log , $\sqrt{}$. It is recommended to always use brackets to ensure the right order of operator evaluation.
- Numbers can be input in various formats, e.g. 1 1. 1.0 1.e00 1.0e+00 . All numbers are treated as double precision regardless of their input format. Likewise, all computations are performed in double precision.
- If desired, an equation-like input can be used, e.g. $\text{mymath}=1+\sqrt{3/2}$. Everything to the left of the equation sign is ignored, only the RHS is used for computation.
- Four variables (not case sensitive) can be used in the expression:
 - ◆ r ...potential radius in fm
 - ◆ en ...c.m. energy of projectile-target system in MeV (for energy-dependent potentials)
 - ◆ c ...Coulomb barrier in MeV
 - ◆ f ...Currently, this is set to be $A^{1/3}$. Caution: The meaning of this variable may change in the future, based on common practice.
- Examples for valid expressions:
 - ◆ $-40 / (1 + \exp((r - 12.5) / 0.62))$
 - ◆ $\text{mypot} = -40 / (1 + \exp((r - 12.5) / 0.62))$
 - ◆ $-4.e1 / (1 + \exp((r - 1.25 * f) / 0.62))$
 - ◆ $(en < 5) * (-100 + 5. * en) + (1 - (en < 5)) * (-75. / (1. + \exp((r - 12.5) / 4.5)))$

Please keep in mind that NON-SMOKER^{web} does not check whether the input functions actually make any sense for an optical potential. It blindly uses the computed values as real and imaginary parts of the optical potential. Unreasonable expressions may lead to unreasonable results or a crash of the code. The latter is just visible by an incomplete result page, explicit error messages are not always shown.

Applicability of the model

Please be aware that the statistical model *may* not be applicable below a certain energy or temperature, although values are given below that limit. The statistical model assumes that averaged transmission functions can be used, i.e. averaging over resonances in the contributing energy window is permitted. At lower excitation energy of the compound nucleus, fewer resonances will be available and thus there may be a lower energy/temperature limit for the application of the model. An estimate of the limiting energy/temperature was derived in a [previous paper](#) and is also explicitly given in [ADNDT 75 \(2000\) 1](#).

The applicability limits can also be checked by calling a result from the [standard result database](#) and looking for possible applicability *warning messages* in the output. (See also the [explanations](#) of the database.) It has to be emphasized that very conservative assumptions are used and that the given results may be valid even below the given limit. The warning is merely issued to point out that one should be cautious and aware of the limitations.

There may be another limitation inherent to all statistical model calculations which do not explicitly include gamma cascades in the compound nucleus. Treating the cascades and the particle escape from the cascade only approximately may lead to larger errors for reactions with negative reaction Q values, i.e. for endothermic reactions. This is not necessarily the case but, in general, for these cases it is safer to calculate the reverse reaction (with positive Q value) and compute the desired reaction by applying detailed balance.

Referencing the results

When using NON-SMOKER^{web} and the linked pages, credit should be given to the [access page](#), the [NON-SMOKER papers](#), and the author. Do not forget to quote the version number you used because different versions may yield different results. The version number is given at the top of each result page returned by the web interface. The desired way of quoting would be, e.g., "...obtained with NON-SMOKER(WEB) v5.8.1w...".

I would appreciate it if a copy of the work is sent to me (e.g. at Thomas.Rauscher@unibas.ch) before publication, so that misconceptions or misinterpretations of the results can be avoided.

Please see also the [disclaimer](#).

Error messages

There are several error messages which can be returned instead of the requested result. They should be self-explanatory. In addition to errors arising from access control or incorrect specifications in the target options, there can be fatal errors when using the customized potential option. These errors will be shown at the end of an incomplete result page and they always refer to a problem with the functions entered in the custom area. Please check your input carefully!

Bug reports

If you encounter a failure or an inexplicable result, please first check the [explanation](#) of NON-SMOKER^{web} and the used methods. Consult the [history section](#) for further details of the current release.

In case you still think that there might be a bug in the returned result, please send a bug report by email, specifying exactly what you did and where you see the problem.

Thomas Rauscher

2. History

24-Aug-2006

This history list is being discontinued. Look in the [forum](#) for information on updates and revisions.

20-Aug-2006

Migration to new server and layout change in the web pages. The function of the code should be unaffected.

01-Jun-2006 to 02-Jun-2006

Server temporarily unavailable due to scheduled power shutdown.

01-Apr-2006

Version 3.3w: Minor changes and bug fixes.

09-Jul-2005 to 11-Jul-2005

Temporarily unavailable due to hardware problem!
Fixed.

15-Mar-2005

1. Version 3.2w: Add Coulomb radius parameter in definition of external potential.
2. Requires new sample input files.
3. New version of checker (Websmokertools Version 2.2) to accommodate the above change.
4. Additional advanced option (deformation).

1-Mar-2005

Version 3.1w: New advanced option and bug fix (specification of external potential).

25-Feb-2005

Version 3.0w: File upload from any directory readable by the user (external file does not have to be in a WWW directory anymore). Some minor bug fixes.

24-Feb-2005

Switched to HTTP POST for sending the form. That means that the result page cannot be bookmarked or linked anymore!

21-Feb-2005

Version 2.01w. Some bug fixes concerning inclusion of experimental masses and custom potentials.

25-Oct-2004

Version 2.0w. Update of experimental masses. Now the experimental and recommended masses from the Audi mass evaluation 2003 are used.

7-Oct-2004

Version 1.1w. New options for custom input file.

22-Sep-2004

Going on-line with version 1.0w!

This version also includes E2 gamma-transitions (the published standard results only use E1 and M1).

© Dr. Thomas Rauscher ([email](#)), last change 2009-Jan-8

Advanced Instructions for NON-SMOKER^{WEB} v5.8w

Custom input file

Advanced options:

The sections ENERGY_GRID and OPTIONS in the NON-SMOKER^{web} input file offer additional flexibility for the experienced user. Use these options with care. You should know what you are doing because changing the default options will offer the possibility to extract additional information while altering (and obscuring) the output of other information at the same time. All options not explicitly set will assume their default values. Without these sections all those options will have the default. Specifying an empty section (i.e. section headers present but no options set within) is not allowed but a whole section can be left out (this is done in the [sample input file](#)). For a sample with all sections, see [the full input file](#).

- **Detailed description:**

- ◆ Energy grid:

- ◇ Section label: ENERGY_GRID

- ◇ If this section is not present, NON-SMOKER^{web} automatically chooses an energy grid of (c.m.) projectile energies which is best suited for integrating the cross sections to obtain the astrophysical reaction rates for the used temperature grid. For instance, a denser grid is used around channel openings where the cross section fluctuates more. When one is only interested in comparing experimental and theoretical cross sections, then it is sometimes better to use a simpler energy grid. When this option is in effect, the code first uses its internal grid for the calculation and then interpolates the results to obtain the values on the specified grid.

- There are two ways to specify different energy grids which are selected by the labels EXPLICIT and GRID, respectively. Those option labels have to appear before the first data in this section.

- ◇ Option EXPLICIT: Energies are given explicitly, one per line, in MeV. Up to 100 energies can be given, if there are more, then the excess values will be ignored.

- ◇ Option GRID: Specification of an energy grid. The order of supplied values is en_start en_step (both in MeV). There can only be one line of this kind.

- ◇ Options EXPLICIT and GRID cannot be mixed.

- ◇ *Note 1: Be careful when plotting these results!* When your step width is too large you may miss certain features of the cross sections (such as fluctuations due to channel openings)! Make sure your step width catches all interesting features. The best is to first make a calculation without this option to identify the energy regions which have to be handled with care.

- ◇ *Note 2:* The S-factors are computed from the original result and then also interpolated (separately from the cross sections). Therefore, there may be small numerical differences between the cross section and its corresponding S-factor at a given energy compared to the "true" S-factor for that cross section.

- ◇ Getting the result page may take longer with this option because the code has to finish all calculations before the interpolation is performed.

- ◆ Further options:

- ◇ Section label: OPTIONS

- ◇ A number of options can be set which affect the results and/or output format. This is only for specialists! Some of the options take 1, 2, or 3 integer parameters which have to be given on the same line as the label. *Note that you must not combine these options with choosing a target range! The results might be incorrect.*

Instructions for NON-SMOKER(web) v5.8w

Currently recognized options include (in alphabetical order):

· COULOMBWF

- # of parameters: 1 (switch=-1...2)
- Select method to compute the Coulomb wavefunctions required for the determination of the transmission coefficients.
 - 1: C. Bardin et al., Comp. Phys. Comm. 3 (1972) 73 (do not use, unstable!)
 - 0: Recursion method by W.R. Smith, Comp. Phys. Comm. 1 (1969) 106
 - 1: Steed's method as implemented by A. R. Barnett 1981
 - 2: (*Default*) Automatic selection of best method as implemented in DFCOUL

· CUTOFF

- # of parameters: 1 (switch=0...2)
- For experts: Cutoff of the gamma width according to its relation to the total width; default value is 1. This is especially important when studying alpha-induced reactions with negative Q-value.
 - 0: cutoff set as in the old SMOKER code
 - 1: (*Default*) different cutoff threshold
 - 2: no cutoff

· DEFORM

- # of parameters: 2 (switch: 0...1, # of lines: 1...4)
- Specify deformations (other than the default ones) for the different channels. The specified deformations are only used if switch>0 (default is 0). The second parameter specifies how many lines with deformation are following.
- This option has to be followed by lines specifying channel and deformation, according to the # of lines given above. The lines have the format '* n x', where '*' can be any of the characters n, p, a, c, 'n' is a switch (0...off (default) or 1...on), and 'x' is the deformation *beta2*. The character at the beginning of the line specifies to which channel/nucleus the given deformation is applied: c...compound nucleus, n...compound-n, p...compound-p, a...compound-alpha.
- Example of a valid entry:

```
#*DEFORM 1 3
c 1 0.283
n 0 0.100
a 1 -0.2
```

In the above definition the deformations for the compound nucleus and the compound minus alpha channel are explicitly given. For the compound minus neutron and compound minus proton (not explicitly given here) channel the default deformations are used.

· E1TRANS

- # of parameters: 1 (switch: 1...6)
- Determines the treatment of the E1 component of the gamma-widths:
 1. Holmes et al. (1976)
 2. Johnson et al. (1977)

Instructions for NON-SMOKER(web) v5.8w

3. Thielemann & Arnould 1983
 4. like 3 but additionally add pygmy resonance (note: this option depends on the treatment of the pygmy resonance currently hardwired in the code and is not applicable to all nuclei; use of this value is strongly discouraged)
 5. GDR energies from P. Van Isacker et al. (1992), Phys. Rev. C45, R13; widths calculated as for 3 but with nuclear properties from ETFSI-2 model (as provided in RIPL-2).
Note: Combining this option with PRINTINFO will not show the correct deformation value!
 6. (*Default*)like 3 but with experimental GDR energies and widths (from RIPL-2), if known
- E2TRANS
- # of parameters: 1 (switch: 0...1)
 - Switch E2 transitions on (switch=1) and off (switch=0) in the calculation of the gamma-transitions. Default is on.
- EQUIVPOT
- # of parameters: 1 (switch: 0...1)
 - Only affecting potentials read from external file: Use deformed potential.
When this option is set the spherical potential is transformed into an "equivalent potential" according to the deformation parameter.
Default value is 1.
- FISSION
- # of parameters: 1 (switch=0...1)
 - Switch fission on (switch=1) or off (switch=0). Default is off.
 - Note: Even when switched on, a nucleus is only considered to be fissionable when there is an entry for fission barriers found in the fission data file! This data file includes the same nuclei as the one calculated by Howard & Moeller 1980 but barriers from a self-consistent Thomas-Fermi model (PRC 60 (1999) 014606) are used.
- FORCEGRID
- # of parameters: 1 (switch=0...1)
 - Use grid specified by ENERGY_GRID also for the internal calculation and do not interpolate. Default is off.
 - This option has no effect when there is no ENERGY_GRID section present and enabled.
 - This option has to be used with care because it can impact the obtained results by changing the integration grid. This is especially true for capture reactions with negative Q-values or photodisintegration reactions in general.
- GDR
- # of parameters: 2 (switch: 0...1, # of lines: 1...2)
 - Specification of GDR parameters when switch=1 (default is Zero). The second parameter specifies how many lines with GDR parameters are following.
 - Without this option or with switch=0, the theoretical description by Thielemann & Arnould 1983 is used (with a low energy modification, see below).

Instructions for NON-SMOKER(web) v5.8w

- This option line has to be followed by one or two (according to the second parameter) lines, each giving a GDR energy and width in MeV. These are the values used for computing the E1 strength in the calculation. If only one line is given, the same values are applied to the GDR part parallel and perpendicular to the axis of symmetry, thus treating the GDR as undeformed (even when the nucleus is deformed). With two lines, the first line gives the energy and width for the parallel collective motion (z) and the second line the ones for the perpendicular motion (xy). (With the `switch` set to Zero, the values are read in but not used; instead the default GDR parameters (e.g., as specified with option `E1TRANS`) are used, which are calculated internally.)
- Note that the GDR used here is not a simple Lorentzian but has a modified energy dependence at low energies. This modification of the low-energy tail of the GDR is also used when the parameters are specified with this option.
- Example:

```
#*GDR 1 2
16.22 5.29
16.22 5.29
```

· ISO

- # of parameters: 1 (`switch: 0...3`)
- Treatment of isospin mixing; it is recommended not to use this option unless you have a very good reason. Currently allowed values:
 - 0: Complete isospin mixing (neglect isospin)
 - 1: Complete isospin mixing but use Woosley et al. suppression factors for gamma width
 - 2: (*Default*) Complete isospin mixing but use Rauscher suppression of gamma width
 - 3: Incomplete isospin mixing (not tested for web use)
 - 4: Incomplete isospin mixing with explicit constant mixing parameter (under construction!)

· MASSOPT

- # of parameters: 1 (`switch: 0...2`)
- Determines how the masses are used to compute the separation energies (Q-values).
 - 0: (*Default*) Experimental masses are taken whenever available, theoretical masses otherwise. However, different masses are not mixed. If there is at least one unknown mass in any of the considered reaction channels, only theoretical masses are taken even when the experimental value is known for a nucleus.
 - 1: Always just use theoretical masses.
 - 2: Always uses experimental masses when known even if mixing of theory and experiment occurs.

Note: This option only affects how Q-values are computed, it does not affect the level density.

· NLDFACT

- # of parameters: 2 (`switch=0...1`, # of lines: 1...4)
- Specify NLD multiplication factors for the different channels. The specified factors are only used if `switch>0` (default is 0). The second parameter specifies how many lines with factors are

Instructions for NON-SMOKER(web) v5.8w

following.

- This option has to be followed by lines specifying channel and factors, according to the # of lines given above. The lines have the format '* n x', where '*' can be any of the characters n, p, a, c, 'n' is a switch (0...off (default) or 1...on), and 'x' is the NLD multiplication factor. The character at the beginning of the line specifies to which channel/nucleus the given factor is applied: c...compound nucleus, n...compound-n, p...compound-p, a...compound-alpha.
- Example of a valid entry:

```
#*NLDFACT 1 3
c 1 2.2
n 0 0.100
a 1 0.2
```

In the above definition the factors for the compound nucleus and the compound minus alpha channel are explicitly given. For the compound minus neutron and compound minus proton (not explicitly given here) channel no factor (i.e. factor=1.0) is used. Only the absolute value of a factor is taken, i.e. any minus sign is ignored.

· NLDAPARITY

- # of parameters: 1 (switch=0...1)
- Determines parity distribution in the nuclear level density as function of excitation energy.
- Switch between equally distributed parities (switch=0) and the parity distribution by Mocelj et al. (2007) (switch=1). Default is the latter.
- Note: The parity distribution chosen here (or the default one) is also used when specifying external parameters for the nuclear level density.

· STATMOD

- # of parameters: 1 (switch=0...2)
- Selects the type of model used to calculate the cross sections and rates. The classical statistical model (Hauser-Feshbach) assumes that the compound nucleus is formed at sufficiently high excitation energy to exhibit all spins and parities. For most stable targets (except at magic numbers) this is a good assumption. However, for astrophysical purposes nuclides with low separation energies have to be considered, in which not all spins and parities are present at a given excitation energy. The (known or calculated) spin and parity distribution, however, can be used to weight the relevant transitions and to compute a suppression factor. This will lead to a suppression of Hauser-Feshbach cross sections for compound nuclei with low projectile separation energy. The value of STATMOD will result in the following behavior:

0: (*Default*) Classical Hauser-Feshbach model (all spins and parities are assumed to occur in the compound nucleus)

1: The compound cross section is weighted according to a parity distribution. Note: This is also affected by the choice in the NLDAPARITY option and other options affecting the

Instructions for NON-SMOKER(web) v5.8w

parity in the nuclear level density.

2: Like 1 but additionally the distribution of the spins with excitation energy is also considered. Note: This is also affected by all options impacting the nuclear level density!

3: (currently disabled) Suppression factor relative to a minimally required NLD

· NUCDENS

- # of parameters: 1 (switch=1...3)
- Select nuclear density distribution used for determining nucleon densities and nuclear radii
 - 1: Local density approximation by Negele, PRC 1 (1970) 1260
 - 2: Droplet model
 - 3: (Default) HFB-02 from RIPL-2

· PRINTINFO

- # of parameters: 1 (switch=0...1)
- Prints some internal values and stops when set to 1. By default, this switch is set to Zero.
- The information printed contains the following:
 - Separation energies in the compound nucleus (in MeV)
 - GDR energy and width in compound nucleus (in MeV); for deformed nuclei, the GDR resonance is split and the values along the symmetry axis (z) will be different from the ones perpendicular to it (xy).
 - For each of the four involved nuclei:
 - EX: can be 1 or 0. A 1 indicates that the mass was taken from experiment, a Zero indicates a theoretical value (the meaning of this depends on the chosen mass treatment).
 - BET: Deformation (beta-Parameter)
 - A: Level density parameter in MeV^{-1} ; when an energy dependent parameter is used, the value at 10 MeV excitation energy is given.
 - DELTA: Backshift of the Fermi-Gas in MeV
 - T: Matching temperature of constant temperature formula
 - E0: Matching energy of constant temperature formula
 - Excited states: The discrete excited states used in the calculation. These are either from experiment or from additional input. Shown is the excitation energy in MeV, the spin, and the parity.

· SENSITIVITY

- # of parameters: 1 (switch: 0...1)
- When switched on (switch=1, default is off), additional output is created, showing the estimated sensitivity to variation of the widths. An additional (required) line gives the desired variation factor f . All widths are consecutively divided and multiplied by the factor f and the sensitivity factors s are printed for each reaction. The sensitivity

Instructions for NON-SMOKER(web) v5.8w

is defined as a real value with a possible range of $0 \leq s \leq 1$, 0 means no change, 1 means full impact of a width variation. In other words, when a width is changed by a factor f the cross section will be changed by a factor $(f-1) * s + 1$ (marked by '=' in the output) or a factor $(1/f-1) * s + 1$ (marked by 'X').

- The sensitivity given is an *estimate* obtained without performing additional variational calculations but rather by comparing the relative size of the widths. For accurate sensitivity studies it is recommended to use the option WFACT to actually vary widths. However, in many cases the estimate obtained here is quite accurate and sufficient.
- Due to the used method it is not possible to estimate the impact of the variation of the width in the entrance channel. Therefore, the results for two assumptions are shown for the width appearing in the entrance channel: 1. The partial (g.s.) width $W_{\text{entrance_gs}}$ is constant while the total width $W_{\text{entrance_tot}} = W_{\text{entrance_gs}} + W_{\text{entrance_excitedstates}}$ is varied; 2. both, $W_{\text{entrance_gs}}$ and $W_{\text{entrance_tot}}$, are varied by the same factor. Case 1 assumes that the total entrance width is dominated by transitions from/to excited target states whereas case 2 assumes that the total entrance width is determined by the transitions from the ground state. For low (astrophysically relevant) projectile energies, often (but not always) case 2 is the better assumption. For a more accurate determination of the sensitivity to a variation of the entrance channel width use the option WFACT.
- Example:

```
#*SENSITIVITY 1
2.
```

This prints an additional section, showing the sensitivities when the widths are varied one by one by the factors 0.5 and 2.

· SPECTRANS

- # of parameters: 3 (switch: 0...4, level_target: 1...(xx), level_exit: 1...(xx))
- Selects a specific transition to be calculated (usually, a sum over all energetically possible transitions is executed). With switch=1-3 the reaction channel is selected (gamma (1), neutron (2), proton (3), alpha (4) channel). The parameter level_target selects the level in the target from which the reaction proceeds and level_exit accordingly specifies the state in the final nucleus in the exit channel chosen with switch. Counting starts with 1 being the ground state, 2 being the first excited state, etc. Predictable results can only be obtained when the addressed states were explicitly input, e.g. by using the section EXCITED_STATES in the input file. A maximum of xx levels (including g.s.) can be specified there, depending on the code version.
- The setting of level_target impacts the calculation even when switch=0! The specified level is treated as the ground state of the target! (The value of level_exit is not used when switch=0).

Instructions for NON-SMOKER(web) v5.8w

- Default values are `switch=0`, `level_target=1`,
`level_exit=1`.
- TEMPGRID
 - # of parameters: 1 (`switch: 0...4`)
 - Redefine temperature grid for the astrophysical reaction rates. Default value is 0. If the MACS are printed, some of them might be incorrect.
- WFACT
 - # of parameters: 2 (`switch=0...1`, # of lines: 1...4)
 - Multiplies chosen widths (transmission coefficients) by a chosen factor.
 - Specify width multiplication factors for the different channels. The specified factors are only used if `switch>0` (*default is 0*). The second parameter specifies how many lines with factors are following.
 - This option has to be followed by lines specifying channel and factors, according to the # of lines given above. The lines have the format '`* n x p s`', where '`*`' can be any of the characters `i`, `n`, `p`, `a`, `c/g`, '`n`' is a switch (`0...off` (default) or `1...on`), and '`x`' is the multiplication factor. The character at the beginning of the line specifies to which channel/nucleus the given factor is applied: `c/g...gamma width`, `n...neutron width`, `p...proton width`, `a...alpha width`, `i...incident width` (between target state MI, usually the ground state). The parity is defined by `p` which can assume values -1, 0, +1 (with 0 transitions from compound states with any parity are used). The spin J of the compound nucleus from which the transition occurs is given as integer value in `s=2*J`. If `s<0`, then all spins (regardless of the value of `s`) are affected and multiplied by the factor `x`, otherwise only transitions originating from a compound nucleus with given spin/parity are multiplied.
 - By mixing `i` and the other options, the transition from the target ground state can be multiplied by another factor than the transitions to the excited target states.
 - Example of a valid entry:

```
#*WFACT 1 3
g 1 2.2 0 -1
n 0 0.100 1 -1
a 1 0.2 -1 3
```

In the above definition the factors for the gamma widths and the alpha widths are explicitly given. For the neutron and proton widths (not explicitly given here) channel no factor (i.e. factor=1.0) is used. Only the absolute value of a factor is taken, i.e. any minus sign in the multiplication factor is ignored.

- WFC
 - # of parameters: 1 (`switch: 0...1`)
 - Switch width fluctuation corrections on (`switch=1`) and off (`switch=0`). Default is on.
- WIDTHS
 - # of parameters: 2 (`switch: -2...2`, `spin: -24...24`)

Instructions for NON-SMOKER(web) v5.8w

- Default value of `switch` is 0 (do nothing). When `switch<>0`: Print averaged widths or strength functions, respectively, for compound states with the given spin/parity. The spin is given in multiples of 0.5, the parity is derived from the sign of the spin parameter. Thus, a value of -3 denotes a $3/2^-$ state. The values are printed for all energies defined by the used energy grid. Averaged neutron, proton, alpha, and gamma-widths are printed when the switch is set to +/-1. Strengths are printed with `switch=+/-2`. For an explanation of the difference of using positive and negative values, see the next item.
- For direct comparison with *experiment* it is recommended to use strengths, not widths. Averaged widths are connected to the strength functions via the nuclear level density, whereas strengths are directly proportional to the potential transmission coefficients internally used in NON-SMOKER^{web}. This is important, for instance, when checking the accuracy of optical potentials against strength functions directly derived from experiment (see [PRC 69 \(2004\) 015803](#)). Another important point when comparing to experimental widths or strength is the impact of the width fluctuation corrections. Those corrections have to be applied when calculating reactions and are therefore used in NON-SMOKER^{web}. For further details, see the above reference and the NON-SMOKER references given elsewhere. However, when comparing to experiment or when publishing resonance data, it is sometimes preferable to quote the *pure* widths and strengths, so that corrections can be applied later when necessary. When specifying `switch=1,2` the width fluctuation corrections are switched *off*. With `switch=-1,-2` the width fluctuation corrections will not be *forced* to be switched off but rather will be on (default) or off (when option `WFC` is given with parameter 0, see below).
- The widths/strength functions are printed for the compound nucleus, i.e. the nucleus made from target+projectile, for the given spin and parity!
- Note that there is a separate column for the entrance channel. The entrance channel column gives the width of the transition to the ground state of the target nucleus, which enters the calculation of the cross section. The other columns show widths summed over all possible transitions.
- For neutrons, also the reduced neutron width and the reduced strength, respectively, are given. Those values are obtained by dividing the neutron width and strength, respectively, by the square root of the neutron energy in eV.

◇ Additional options might be added to this section without further notice...

• Final remarks

- ◆ Do not forget to check your input file with the [checker tool](#). However, [that program](#) does not check the validity of the options within the `OPTIONS` section!
- ◆ Because of the complexity of the options and the sensitivity of the results to them, please check carefully what you are doing and do not hesitate to consult the author by EMAIL!

© Dr. Thomas Rauscher ([email](#)), last change 2009-Jan-8