MUCAT
manual

MUCATEX, 2003.

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Contents.

1. Introduction

The present Manual is the guide onthe usage of the program MUCAT, created for description of kinetics of muon catalyzed fusion (μCF) processes in mixtures of hydrogen isotopes. It enables simulation of μCF phenomenae under in conditions of hydrogen mixtures in theoretical research, and also for analysis of experimental data.

The MUCAT code is based on the Monte-Carlo method of simulation of real trajectories, , intended for calculations of populations of different states and the yields of reactions in specified intervals of energy, time or coordinates in assumption that the rates (either constant or dependent on energy()) of μCF reactions are known.

The input data, such as the cross sections and the rates of μCF processes can be easily corrected and updated with any new available data. The user can set an arbitrary kinetic scheme of his choice (in particular, the states may be not only muonic, but also e.g. pionic), the media composition and 2D-geometry (see the section 4). The code supports the energy-dependent reaction rates and cylindrical geometry of media.

The method and the earlier versions of the code have been tested on the data analysis of the experiments [1-5] and provided extraction of the main characteristics of μCF processes. The first calculations based on this code with energy-independent cross-sections had provided a qualitative agreement with the results of the PSI-89 experiment on μCF in triple mixtures of isotopes H/D/T with low concentrations of D and T [1]. By varying several rates, the quantitative agreement has been achieved. The first calculations with 2D-geometry were used in [2].

The program code MUCAT is written in FORTRAN-77. Its present version of FORTRAN code takes about 240 KB of disk storage and in addition to it approximately the same space takes the cross-section library, which may be extended as needed. A minimum value of RAM, which is necessary for the code running, is about 550 KB. It depends on complicity of the kinetic scheme and volume of the information required for out-printing. The calculation of 10^5 muon evolutions at 0.05 LHD target density according to the Test Run (Appendix B) on a PC with 1410 MHz AMD processor takes about 3.3 minutes, but the calculation of cross sections CMS→LAB takes about 30 minutes in the same example. It is recommended to set the number of muons to $10^4 \div 10^5$ for fast tests, and 10^6 muons for calculations with higher accuracy. At 10^6 muons the accuracy is usually sufficient for comparison with experimental data.

2. Formulation of the problem and the scheme of solution

Suppose that there is an infinite target, being a homogeneous mixture of hydrogen, deuterium and tritium. A muon stops in this media, and produces a series of μCF cycles. A muon cycle is a chain of events that occurs with the muon between its two consecutive free states. A series of muon cycles is defined here as a number of events from the initial state to leaving a cycle due to muon decay, sticking or leaving the target volume.

Considering series of μCF cycles, we shall always trace the muon, and call his bound states with molecules and atoms the states of muon, or μ-states. We shall refer to the kinetic energy of such a composition as to the energy of the μ-state. Every reaction, in which the μ-states takes place, we call a transition. A transition may occur either with a change of state, such as decay, fusion, excitation, or without change, in the elastic scattering.

A typical scheme of μCF cycles in a triple mixture of hydrogen isotopes is shown in the Fig.1. The circles are the μ-states, the arrows are the transitions. The rectangles are the states, that terminate the series of μCF cycles. For all circles the transitions corresponding to the muon decay and the elastic scattering are implied but not shown on the scheme.

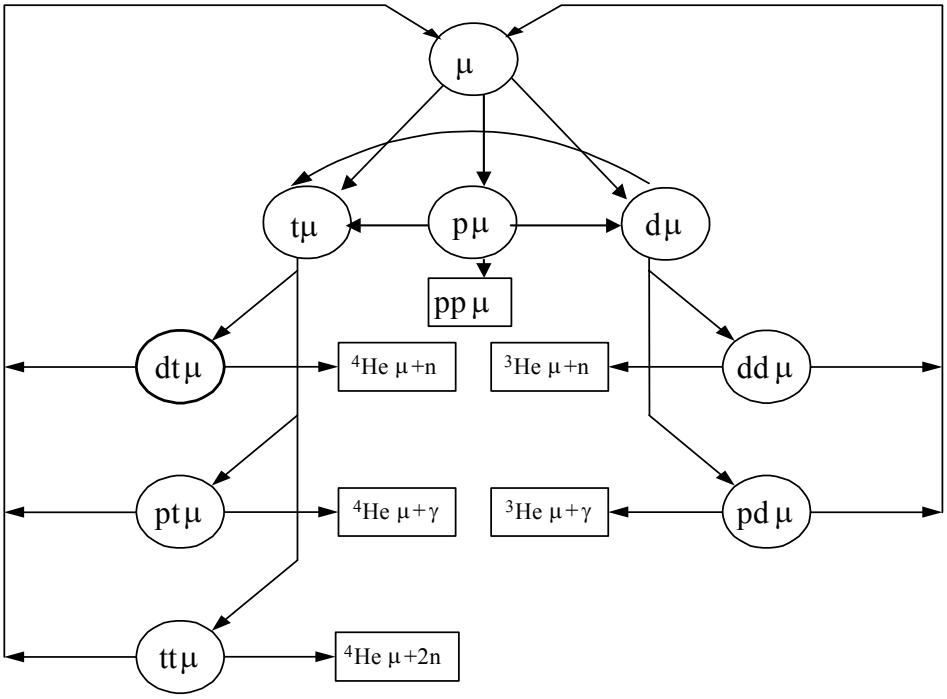


Fig.1. The kinetic scheme of MCF processes in a triple mixture of hydrogen isotopes.

More or less detailed kinetic schemes are possible. For example, the state pμ may be represented as two states with different spins, pμ(0) and pμ(1). Then we have to change the node of the Fig.2a to the following two nodes of Fig.2b.

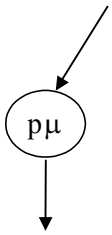


Fig.2a

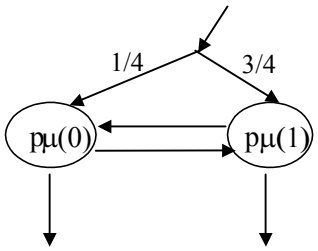


Fig.2b

To include a calculation of an atomic cascade, no code modification is required. The cascade transitions occur between excited states of mesic atoms, which are normal kinetic states for the code. So for a cascade calculation, one has to describe an appropriate kinetic scheme and include necessary files into the cross-section library, to specify the transition rates.

Having described the set of all states and all rates of transitions between them, it is possible to calculate populations of the states and reaction yields. (A population of a state means how many muons are in that state at the moment, and a reaction yield means how many reactions occur for one muon). The MUCAT code does this, simulating the processes by the Monte-Carlo (MC) method. To generate events by the MC method, one has to define:

1) the kinetic scheme – the possible μ-states and the transition rates between them,
2) the initial state and its energy,
3) the target media composition, temperature and geometry.

Tracing the evolution of every muon, we know at any moment its state, energy, coordinates and the direction of movement. At a state with definite energy the rates of all possible transitions are calculated. The transition channel and the corresponding final state are chosen using a random number. Then the time of the next interaction is calculated. After that the event is added to the event counter. If the final state of the next transition is present in the list of requested distributions, the corresponding event counter is incremented by one. Otherwise, nothing is incremented.

If the user has requested, for example, an energy distribution of a population of some state at some appropriate moment of time, then the check is performed, whether this moment is between the two sequential transitions. If yes, then the number of energy bin of the requested distribution is calculated, and this bin's contents is incremented by one. In this way the program counts all the events of interest. To obtain statistics, a large number of muons is traced. Every muon takes part in one series of μCF cycles.

The simplified MC algorithm is shown on the Fig.3, with the following steps:

- initialization (setting the muon to the initial state, energy and direction of motion, and setting the current time to t=0);
- calculation of the muon decay moment T_{dec};
- random generation of the reaction parameters: the time interval before the next interaction T_{int}, the final state, the transition channel and the interaction coordinate;
- calculation of the contribution of this last interaction to the requested distributions of populations and reaction yields (incrementing corresponding bins and counters);
- calculation of the contribution to the total yield;
- determination of the new kinematics (the energy and direction of motion) of the μ-state;
- return to calculation of condition of the next transition.

If the muon decay occurs ($t > T_{dec}$) or the current time exceeds the maximum time in requested distributions T_{max}, then the new series of cycles starts for a new muon, beginning from the initial state.

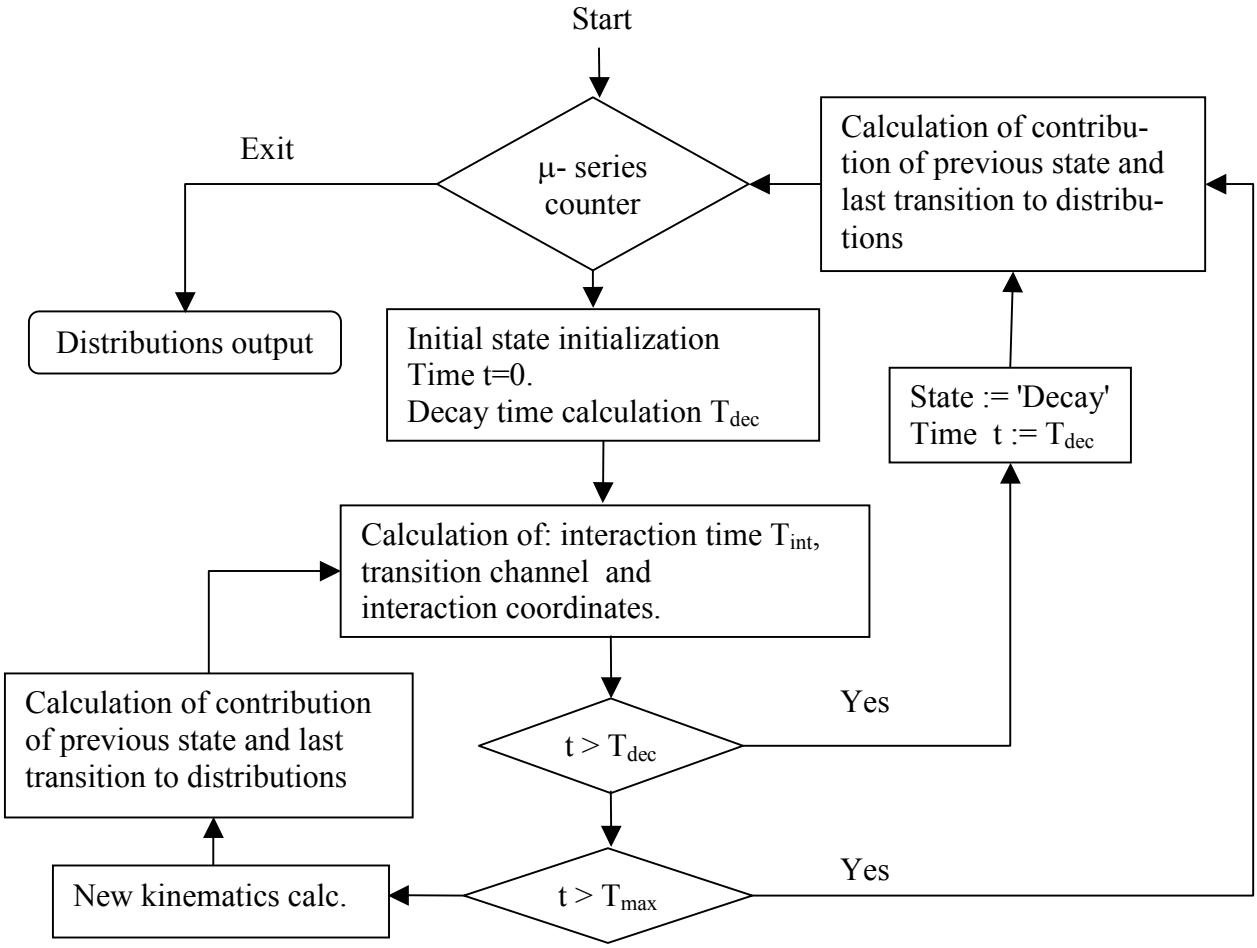


Fig.3. Monte-Carlo calculation algorithm.

3. The code structure

The Fig.4 shows the functional block scheme of the computer code. To run the *Executable Module*, the following *input data* must be arranged: the Kinetic Definition File, which determines the kinetic scheme, the library of cross-sections (Cross-Section Files) and the number of muons (Number of μ series).

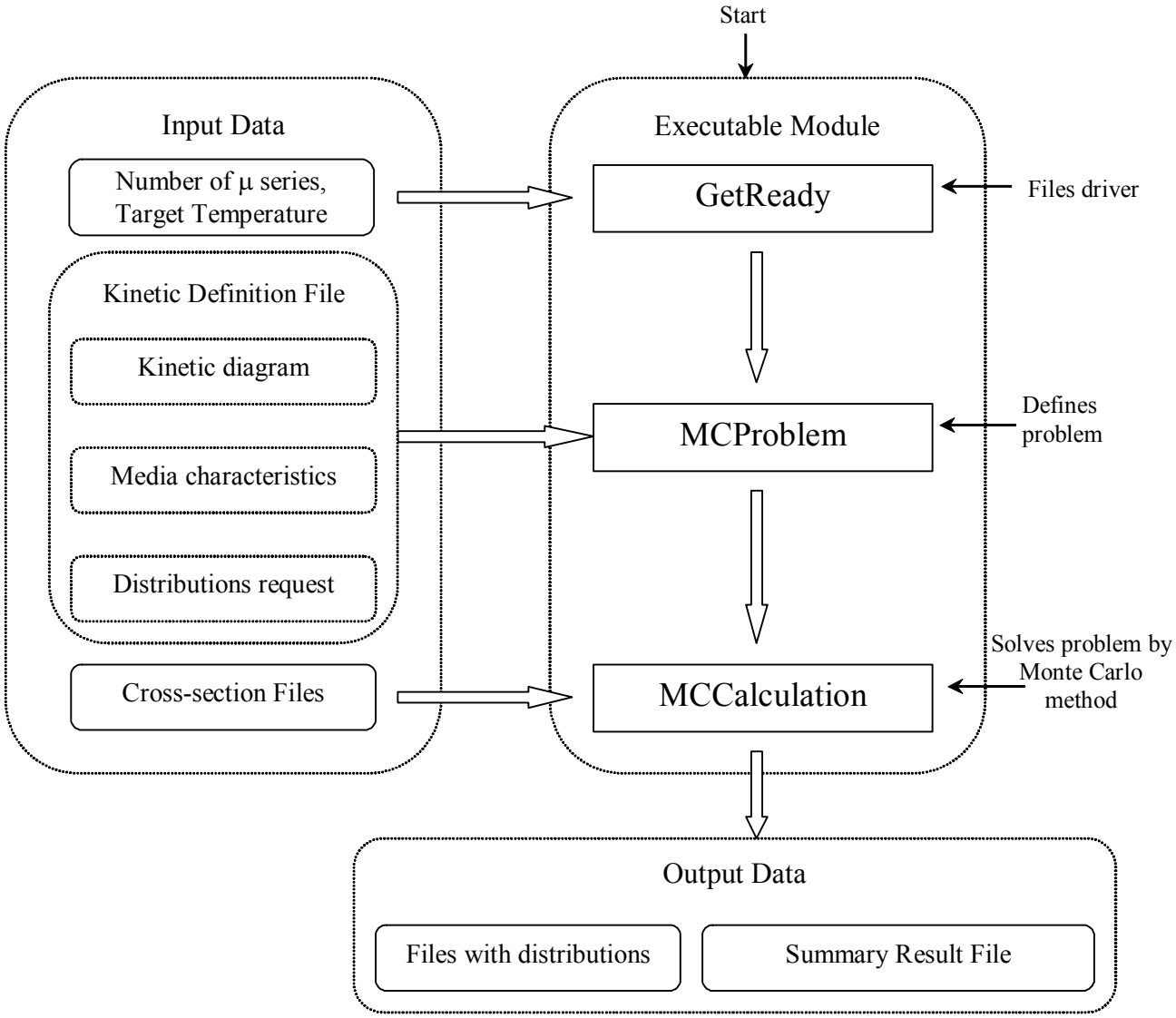


Fig. 4. Functional block diagram of the computer code

The *Number of μ series* is prompted immediately by the starting program, to be input from the keyboard. (See an example in the Test Run; some recommendations on the Number choice are in the Introduction). The Target Temperature is entered in the same way as the *Number of μ series*, but only in that case when the double differential cross-sections have to be obtained (see the section 5, the "Hot media" model).

In the *Kinetic Definition File* the user has to define the kinetic scheme (possible μ-states and transition rates between them, and the initial state), the media properties (target's components densities in units of Liquid Hydrogen Density), some auxiliary information (used for monitoring and control), and the request for output distributions.

The *Cross-Section Files* comprise the cross-section library. Their names have to be indicated in the Kinetic Definition File at setting of the kinetic scheme. These files define the transition rates, dependent on the state energy. They contain information about the masses of particles, taking part in the reaction, the angle and energy distributions of the final particles of transi-

tions. The Cross-Section Files, describing the muon stop in the target at its capture by media particles, contain also the information about the spatialboundaries for the muonic atom formation. The processes at different media temperatures are described by their specific files of the cross-section library.

The Output Data are composed by the program according to the requests in the Kinetic Definition File. Those requests may be for various distributions of states populations and reactions yields. Every distribution is output as a single file. Their names are also defined in the Kinetic Definition File. Moreover, *Summary Result File* with some service information and integral characteristics is output. See details in the Section 3.2.

The *Executable Module* consists of the three principal subroutines: GetReady, MCProblem, MCCalculation (Fig.3). They are called from the main program MUCAT.

GetReady does the preliminary operations: it opens the kinetic definition file, sets the units of physical quantities, prompts for the number of muons, opens the output resulting file.

MCProblem reads the kinetic scheme and defines the problem that is to be solved, that is the requested distributions.

MCCalculation solves the problem by Monte Carlo method, using the cross section library and writes the results into *Output* files.

3.1 The structure of the Kinetic Definition File

The user can modify this file by any text editor. It contains FORTRAN-readable records. Every line contains a fixed number of items, and therefore may be appended by arbitrary comments. Here is an example of Kinetic Definition File C:\Mucat\Run \Test\Hot.kin, which is used for the Test Run and describes thermalisation of dμ-atoms in gaseous D_2.

```
'*TITLE' Hot.kin Deceleration and spin-flip of mud in D2 without mudd formation
 'Hot.kin'
'*SHOW'
      3
'*PARAMETER'
      'CD'
      'Zmin'
      'Zmax'
      'Ethermal'
      'Z1'
      'Z2'
      'END'
'*LET'
      'CD'    0.1        LHD
      'Zmin'   1.e-6      mm, Compact source
      'Zmax'  -1.e-6
      'Ethermal'  0.5       eV, below is the new algorithm
      'Z1' -10.          mm
      'Z2'  10.
      'END' 0.
'*MEDIA'
      'D2Gas '
      'END'
'*VOLUME'
      'Target' 'D2Gas ' 'Z1' 'Z2'
      'END' 'END' ' ' ' '
'*STATE'
      'mu'
       'mud1'           initial energy  E = 1.0 eV
       'mud2'
      'END'
'*INITIAL'
      'mu'
```

```
'*LINK'
   'mu' '->' 'mud1' 0.3333E8   'Mud_e1'       1/3
   'mu' '->' 'mud2' 0.6667E8   'Mud_e1'       2/3
      'mud1'  '->'  'mud1'  1.  'dd11'
      'mud1'  '->'  'mud2'  1.  'dd12'
      'mud2'  '->'  'mud1'  1.  'dd21'
      'mud2'  '->'  'mud2'  1.  'dd22'
      'END' '->'  'END'     0.    'END'
'*DECAY'
      0.455   Decay rate in units of 1/mks
 '*TIME'      Maximum time
      20.
 '*RADIUS'
       1.
'*POPULATION'
   'mud1'   'Energy'  0.002  0.0 1.2 0.01   0. 0.   'mud1e2'
   'mud2'   'Energy'  0.002  0.0 1.2 0.01   0. 0.   'mud2e2'
   'mud1'   'Energy'  0.03  0.0 0.2 0.001   0. 0.   'mud1e30'
   'mud2'   'Energy'  0.03  0.0 0.2 0.001   0. 0.   'mud2e30'
   'mud1'   'Time'     0.   0.0 1.275 0.005   0. 0.  'mud1t'
   'mud2'   'Time'     0.   0.0 1.275 0.005   0. 0.  'mud2t'
   'mud1'   'Time'     0.   0.0 1.275 0.005  0. 0.1  'mud1tw01'
   'mud2'   'Time'     0.   0.0 1.275 0.005  0. 0.1  'mud2tw01'
   'END'    'END'    0.    0. 0. 0.00  0. 0.   'END'
'*YIELD'   Calculated distributions
  ' '  '->' 'ESCAPE'  ' '  'Energy'   0. 0.25 0.005  0.0 0.0   0. 0.  'EscE'
  ' '  '->' 'ESCAPE'  ' '  'Energy'   0. 0.25 0.005  10. 20.  0. 0.  'EscEw'
  '  ' '->' 'DECAY'  ' '  'Time'    0. 5.0  0.05   0.0 0.0   0. 0. 'DecT'
  '  ' '->' 'DECAY'  ' '  'Range'    0. 1.0  0.01   0.0 0.0   0. 0. 'DecR'
  '  ' '->' 'DECAY'  ' '  'Range'    0. 1.0  0.01   1. 10.  0. 0.04 'DecRw'
 'END'  '->'  'END'  'END'  'END' 0. 0. 0.  0. 0.  0. 0. 'END'
 '*END'   End of kinetics definition
```

****

The Kinetics Definition File consists of the following mandatory sections.

1. The name of the Kinetics Definition File
2. The list of parameters
3. The list of parameter values
4. The list of states
5. Indicator to the initial state
6. The list of transitions
7. Muon decay rate
8. Maximum duration of one muon series
9. The list of the requested results to be output.

Every list begins by an indicator – the list header. It is a character constant, beginning from the symbol '*'. The list has to be terminated by the constant 'END', except of the case when it is a simple list with fixed number of items. For example, the record of the file title contains two lines and has the following format:

'*TITLE' — indicator

'Filename' — the name of the processed file 'Filename.kin'

According to the example of a Kinetics Definition File on the page 6, 'Filename' = **'Hot.kin'**.

There are also the following simple lists there:

the muon decay rate

'*DECAY'

0.455 — in units 10^6 of s^{-1};

the initial state indicator

'*INITIAL'
'Name_1' — one of the names from the list of states;

and also the maximum duration of one muon series (this is an auxiliary constant, used to prevent infinite looping in case of a too long value of muon lifetime; if it is set to be large enough, it has no effect on results)

'*TIME'
20. — in units of 10^{-6} s.

The simple list with the indicator '*SHOW' in the example sets the level of debugging information to be displayed on the screen and written into the file of results. It has to be followed by one of the numbers 0,1,2 or 3. If it is 0 or if the list is absent, the information is not output.

The system states are identified by their names – character constants, this provides readability and avoids necessity of manual numbering. The list looks like this (with names in brackets as in the example on page 6)

'*STATE' — the list header
'Name_1' — the first name ('mu')
'Name_2' — the second name ('mud1')
…
'Name_n' — n-th name
'END' — end of the list.

Here it is not allowed to use the names 'DECAY' and 'ESCAPE', corresponding to muon decay and to its escape from the target.

The **kinetic scheme** is determined by the list of transitions, which is of the following format:

'*LINK' — the header of the list
'Name_1' '->' 'Name_i' const_1 'Fname_1'
…
'Name_n' '->' 'Name_n' const_n 'Fname_n'
'END' '->' 'END' 0. 'END' — the end of list .

In every line of the list the user has to indicate the name of the initial state of the transition (it is a character constant before the arrow '->'), the name of the final state (the character constant after the arrow), the statistical weight of the final state (const_i) and the name of the file (Fname_i.fcn), where the reaction rate and the reaction parameter, included in the parameter list, are written. For example, if in the file Fname_1.fcn there is the constant 'CD' as a parameter, meaning the deuterium density, then this means the transition in interaction with protium. The reaction rate in this channel is taken from the file Fname_1.fcn and multiplies to the value of the parameter ('CD' for this example) and to the value const_i. If the filename is blank, the rate is considered to be const_i (in units 10^6 s^{-1}). Instead of the file name there may stand a parameter of density, 'CD' for example. Then, as previously, the rate is const_i (in units 10^6 s^{-1}) multiplied the parameter value. (The last case is processed by the Subroutine KFCN0).

If we want to control the transition of the muon to the next catalysis cycle, we have to introduce the new state, e.g. 'next', and the parameter 'REC', and in the list of transitions we have to split the line, that is like this:

'n+3He+mu' '->' 'mud' …

into two lines like this:

'n+3He+mu' '->' 'next' 1.e8 ' ' recycling
'next' '->' 'mud' 1.e8 'REC'

At the zero value of the parameter 'REC' the muon series terminate after one muon cycle.
The following example of '*LINK' list (see Table 1) corresponds to the kinetic scheme of the Fig.1.

Table 1. Kinetic definition file fragment corresponding to Fig.1.

The line in kinetic file	Comment

'*LINK'	List header
'mu' '->' 'mup' 1.e8 'Mup_e1'	Muon capture: μ+p → pμ
'mu' '->' 'mud' 1.e8 'Mud_e1'	Muon capture: μ+d → dμ
'mu' '->' 'mut' 1.e8 'Mut_e1'	Muon capture: μ+t → tμ
'mup' '->' 'mup' 1. 'Mup_p11'	scattering: pμ+p → pμ+p
'mud' '->' 'mud' 1. 'Mud_p'	scattering: dμ+p → dμ+p
'mud' '->' 'mud' 1. 'Mud_d11'	scattering: dμ+d → dμ+d
'mut' '->' 'mut' 1. 'Mut_p'	scattering: tμ+p → tμ+p
'mut' '->' 'mut' 1. 'Mut_d'	scattering: tμ+d → tμ+d
'mut' '->' 'mut' 1. 'Mut_t11'	scattering: tμ+t → tμ+t
'mup' '->' 'mud' 1. 'Tr_pd'	Muon transfer: pμ+d → dμ+p
'mup' '->' 'mut' 1. 'Tr_pt'	Muon transfer: pμ+t → tμ+p
'mud' '->' 'mut' 1. 'Tr_dt'	Muon transfer: dμ+t → tμ+d
'mup' '->' 'mupp' 1. 'Ppmu'	Muonic molecule formation: pμ+p → ppμ
'mud' '->' 'mudd' 1. 'F12_d_3'	Muonic molecule formation: dμ+d → ddμ
'mud' '->' 'mupd' 1. 'Mf_pdmu'	Muonic molecule formation: dμ+p → pdμ
'mut' '->' 'mudt' 1. 'F1_d_3'	Muonic molecule formation: tμ+d → dtμ
'mut' '->' 'mupt' 1. 'Mf_ptmu'	Muonic molecule formation: tμ+p → ptμ
'mut' '->' 'mutt' 1. 'muttmutt'	Muonic molecule formation: tμ+t → ttμ
'mudd' '->' '3Hemu+n' 1.e2 ' '	fusion: ddμ → ^{3}Heμ+n
'mudd' '->' 'mu' 1.5e3 ' '	fusion: ddμ → ^{3}He+μ+n
'mupd' '->' '3Hemu+g' 5.e-2 ' '	fusion: pdμ → ^{3}Heμ+γ
'mupd' '->' 'mu' 8.e-1 ' '	fusion: pdμ → ^{3}He+μ+γ
'mudt' '->' '4Hemu+n' 6.8e3 ' '	fusion: dtμ → ^{4}Heμ+n
'mudt' '->' 'mu' 1.2e6 ' '	fusion: dtμ → ^{4}He+μ+n
'mupt' '->' '4Hemu+g' 1.e-2 ' '	fusion: ptμ → ^{4}Heμ+γ
'mupt' '->' 'mu' 1.0 ' '	fusion: ptμ → ^{4}He+μ+γ
'mutt' '->' '4Hemu+2n' 1.3e1 ' '	fusion: ttμ → ^{4}Heμ+2n
'mutt' '->' 'mu' 0.3 ' '	fusion: ttμ → ^{4}He+μ+2n
'END' '->' 'END' 0. ' '	End of the list. The first word must be 'END'

The list of parameters has the title '*PARAMETER'. It must contain the concentrations and other parameters, written in the files with the extension *.fcn, for example, the values 'Zmin' and 'Zmax', corresponding to the spatial limits of muon stop area in the target. In the example file above, Hot.kin, these limits are used for calculation of dμ-atom coordinates after a muon capture, described by the file C:\Mucat \fcn \fcn_4\Mud_e1.fcn. The presence of the parameter 'Ethermal' in this list means that the "Hot media" model is implemented. Absence of this parameter says to use the "Cold media" model only.

Values are set to the parameters in the list of parameter values, which looks like

'*LET' — the header
  'Namepar1' Value1
  …
  'NameparN' ValueN
'END' 0. — End of the list.The densities are given in units of liquid hydrogen density (1 LHD = $4.22 \cdot 10^{22}$ cm^{-3}), the coordinates — in mm. The value of the parameter 'Ethermal' (in units of eV)

stands for the boundary energy of a μ-state, below this energy the "Hot media" model is implemented. To exclude the "Cold media" model completely, the thermal parameter should be made large enough: higher than the edge of the energy grid applied for hot-media-model calculations. For the applied 101-point grid (see section 5.1) this edge is 105.75 eV. At zero value of the thermal parameter, the "Hot media" model is excluded completely.

The list of output results may be in one of the two forms, one corresponding to the populations of states and the other to the numbers of events. The list of populations can request to output various distributions of populations. This list has the form

'*POPULATION'
  'Name' 'Type' A Bmin Bmax Bstep Cmin Cmax 'Fname'
  …
'END' 'END' 0. 0. 0. 0. 0. 0. 'END'

Here 'Name' is the name of the state to display the population of; 'Type' is the distribution type that can be 'Energy' or 'Time' for energy and time distributions respectively. The constant A defines the moment of time to calculate the population at. The constants B and C are either energies or times respectively, they are the limits of the distribution. The file name 'Fname' will be used to create the output file Fname.dat with the requested distribution. In the first column the values of B are printed, from Bmin to Bmax with the step Bstep (the maximum number of intervals between [Bmin,Bmax] is not allowed to be more than 256). The second column contains the populations of the state. For time distributions (of type 'Time') the constant A is ignored, and the constants B are taken as the limits of the time interval from Bmin to Bmax with the step Bstep, in units of microseconds.

The constants Cmin, Cmax define the energy interval [Emin,Emax] in the units of eV. If both constants are 0, then the energy interval is unlimited. For the energy distributions, the constants C are ignored, e.g.

'mud1' 'Energy' 0.002 0.0 1.2 0.01 **0. 0.** 'mud1e2'

Here 'mud1' is the name of a state, which may correspond to $d\mu_{1/2}$; A = 0.002 mks — the moment of time, when the population is calculated, Emin = 0. eV, Emax = 1.2 eV, Estep = 0.01 eV. Thus, this population corresponds to the energy distribution of $d\mu_{1/2}$ -atoms at 2 ns after a muon stop in the target.

For every distribution, supplementary constraints can be imposed by setting time and energy windows. (There is no sense to set, for example, an energy window for the energy distribution). The reaction yield list can serve for these and other purposes:

'*YIELD'
 'Initial' '->' 'Final' 'Transition' 'Type' Bmin Bmax Bstep Tmin Tmax Emin Emax 'File'
 …
 'END' '->' 'END' 'END' 'END' 0. 0. 0. 0. 0. 0. 0. 'END'

'Initial' and 'Final' are the initial and final states, which define the event. The event may be defined or restricted also by the transition 'Transition' (it can be a file name without extention, which defines the transition, e.g. 'mup_p11') or by only one of the states. Distributions can be, besides 'Energy' and 'Time', also of other types, e.g. 'X', 'Y' and 'Z', which correspond to the distributions along the coordinates X, Y or Z, 'Range' – the distance from the starting point of the catalysis: $\sqrt{X^2 + Y^2 + Z^2}$, and also 'cos' – the distribution over the cosine of the angle between Z-axis and muon direction.

Other data are similar to the populations list. The energy values correspond to the initial state. An example:

' ' '->' 'DECAY' ' ' 'Range' 0. 1.0 0.01 1. 10. 0. 0. 'DecRw1'

'Initial' = ' ' — blanc means any initial state,

'Final' = 'Decay' — the state "muon decay",
'Transition' = ' ' — blanc means "anything that leads to decay",
'Range' 0. 1.0 0.01 — (in mm) defines the distribution,
1. 10. — defines the time window (selects only the events that take place between 1 mks and 10 mks)

If a distribution is required of the same type but only for decays from the states with energies between 0 and 0.04 eV, then the following line should be added to the reaction yield list:

```
'  ' '->' 'DECAY' ' ' 'Range'   0. 1.0  0.01   1. 10.  0. 0.04 'DecRw'
```

The kinetic setting is terminated by a simple indicator '*END'. The order of indicators is almost arbitrary, but '*LET' must not appear before '*PARAMETER', and '*STATES' must stay before '*LINK', '*POPULATION' and '*YIELD'.

The lists **'*MEDIA'** and **'*VOLUME'**, as well as **'*RADIUS'**, are implemented for the target geometry setting and described in the section 4 "Target Geometry".

3.2 The structure of the cross-section library

The set of cross-section files is the library, composed in advance, which is mandatory for calculation of transition rates and kinematics of the final state of every reaction. For every type of interaction there is a special file type with appropriate data arrangement (we call it a class) and a special subroutine that processes this data. The first 6 characters in the first line of the file specify the file class. In the following table one can see the correspondence between the file class and the subprogram name.

Table 2. List of file classes

Identifier	Subroutine name	Comment
'1->2 '	KFCN12	Muon capture
'1->2 W'	KFCN12W	Muon capture
'1->2 R'	KFCN12RW	Muon capture
'2->2 '	KFCN22	scattering
'2->2Z '	KFCN22Z	scattering
'2->2 T'	KFCN22T	scattering
'2->2W '	KFCN22W	scattering
'2->2DZ'	KFCN22DZ	scattering
'2->1 '	KFCN21	Muonic molecule formation
'2->1RS'	KFCN21RS	Muonic molecule formation

As it is shown in the Table 2, at present there are 10 classes of data files, which differ in general by the number of particles in initial and final states of reactions. The data in a file specify:

- the class identifier,
- the interaction parameter (the target particle),
- masses of particles,
- reaction rate (dependent on energy)
- In several classes there is the angular distribution of scattered particles as a set of polynomial coefficients.

In all data files the cross-sections and rates are averaged over the rotation and vibration states of media molecules at certain temperature. Therefore different data files correspond to different temperatures.

The class '2->2 ' describes the scattering of a muonic atom or a molecule on the particle of a media. In general, this class describes any reaction, in which there are two particles in the initial and 2 particles in the final state. Below is a file of this class that corresponds to elastic scattering of pμ-atoms with spin 0 on protons.

```
'2->2   ' Deceleration mup(0)+p->mup(0)+p          File 'mup_p11.fcn'
'CP     '    5                  T=30K  OCT-1996
1043.93e6  938.272e6  1043.93e6  938.272e6  0.0   0.04 100.
 0.001   110.    0.5  0.001 0. 0. 0.
 0.002   155.    0.5  0.001 0. 0. 0.
 0.003   190.    0.5  0.001 0. 0. 0.
 ...
```

Here **'2->2 '** is the class identifier. The 7-th character of the first line we call 'label'. In this example, the label is blank **' '** .

'CP ' is the multiplicative parameter of this class; it defines the density of those particles of the media the scattering occurs on. This parameter must be declared in the Kinetic Definition File and its value must be set there in the list '*PARAMETER'.

In the same line with the multiplicative parameter there stands the integer number N, corresponding to the power of the polynomial approximation of the scattering angle distribution (see below). In the example above N = 5.

The rest of the line is filled with comments. In this example temperature T=30K corresponds not to the Maxwellial motion of target particles, but to the population of rotational states of H_2 molecule.

The third line

```
1043.93e6  938.272e6  1043.93e6  938.272e6  0.0   0.004 100.
```

contains the masses of particles (M_1 M_2 M_3 M_4), the energy outcome of the reaction (ΔE, if the energy is absorbed, then it goes with minus sign), and the limits of the distribution. All the values are in eV units. Thus the third line corresponds to the following:

M_1 M_2 M_3 M_4 ΔE E_{min} E_{max}.

For the "Cold media" model the value E_{max} is not used and E_{min} has different meaning, dependent on the label. If the label is blank or **'S'**, or **'X'** and is implemented, then all the states, that had obtained energy less than E_{min} after the interaction, are assigned to have this fixed energy E_{min}. If the label is **'Z'**, then the reaction rate is considered to be zero at interaction energies below E_{min}. For the other details in the meaning of E_{min} and E_{max}, see the section 5 "Hot media model".

The rest of the file is the table of the form:

Energy Rate C_1 C_2 C_3 ... C_N

Where Energy is the collision energy in the center of mass system.

The angular distribution of scattered particles in the center of mass system is

$$\frac{d\sigma}{d\Omega} = \frac{\sigma^{total}}{2\pi} \sum_{n=1}^{N} C_n \cos^{n-1}\theta$$

with normalization

$$1 = \int_{-1}^{1} \sum_{n=1}^{N} C_n \cos^{n-1}\theta \quad \mathrm{d}\cos\theta \,.$$

Depending on the label (' ', 'I', 'L', 'S', or 'X'), the value Rate has different meaning

Table 3. List of labels for the class '2->2 '.

Label	' '	'I'	'L'	'S'	'X'
Meaning of the 'Rate'	Reaction rate in units mks^{-1}	The same, but the program stores and interpolates	The program interpolates Lg(Rate)	Reaction rate (mks^{-1}), divided by the μ-particle velocity (in units	σ^{total} in units cm^2

		1/Rate		of light velocity c)	

Now consider another class of files, describing the muonic molecules formation. They have the following structure

'2->1 ' [Comment: or '2->1 L ', if ln(y) is to be interpolated,
or '2->1 I ', if 1/y is to be interpolated,
or '2->1 0 ', if Elab=Vlab=0 after the reaction; in all other cases
Elab and Vlab are unchanged]
'Par_Name' E_cut_min E_cut_max [Comment]
Energy Rate [Comment]
... ...

Here one can set not more than 250 energy points. The μ-state energy Energy is in eV and Rate is in units mks^{-1}. If the energy is out of the range (E_cut_min, E_cut_max), then the rate of the reaction is set to be 0.

For example, the file F0_D_3.FCN:

```
'2->1  0 '  dtmu formation mut(0)+D2(T=3K),  molecule stops.    1994
 'CD2    '  0.  3.           LHD    File F0_D_3.FCN
      0.0004   8.918E-02
      0.0008   1.307E-01
      0.0012   1.717E-01
      ........      ............
      2.9100   7.984E-02
      2.9500   5.846E-02
      2.9900   5.203E-02
```

This file describes the energy dependence of dtμ molecule formation at temperature 3K in collisions of tμ(0) with the molecule D_2, with concentration determined by the value of parameter **'CD2 '**. The velocity of the formed muonic molecule is set to 0, this is indicated by the label **'0'** in the class identifier. At the collision energy over 3 eV, formation does not occur.

The file for description of muon capture looks as follows:

'1->2 W H' [Comment] - the identifier of the given class ('H' — is the label)
'Par_Coef' [Comment] - multiplicative parameter for the rate
Rate [Comment] - coefficient for the rate
Mass [Comment] – mass of the formed particle
'Zmin' [Comment] - parameter for the lower boundary of muon stop area
'Zmax' [Comment] - parameter for the upper boundary of muon stop area
COSmin [Comment] - $COS(\theta_{min})$
COSmax [Comment] - $COS(\theta_{max})$
PHImin [Comment] - φ_{min} — minimum azimuthal angle of the outgoing particle
PHImax [Comment] - φ_{max}— maximum azimuthal angle of the outgoing particle
E1 W1 |
E2 W2 | — energy distribution of muonic atoms
... |
ENmax WNmax |

The position in space is redefined, if 'H' ='Z'.

For example,

```
'1->2 W Z'          Atomic capture mu->mup       mup_E10.FCN  July 1999
 'CP     '          ***  Limited z-range  ***
  1.e7                      ***  Isotropic       ***     Very Fast ***
  1043.93e6    ***  Delta  1.00 eV  ***
  'Zmin   '
```

```
'Zmax    '
-1.
 1.
 0.
 6.28318
    0.    0.
    0.999 0.
    1.000 1.
    1.001 0.
    2.0   0.
    10.   0.
```

The values of parameters **'Zmin'** and **'Zmax'** are set in the Kinetic Definition File, they define an area where muon stops in the target. θ_{min} and θ_{max} are the minimum and maximum polar angles of the formed and outgoing muonic atom, with respect to Z axis, which is directed along the muon beam. In this example $\cos(\theta_{min})= -1$, $\cos(\theta_{max})=1$, and the azimuthal angle $\varphi_{min}=0$, $\varphi_{max}=2\pi$ corresponds to isotropic distribution of muonic atoms. Their energy distribution is sharply peaked at 1 eV of muonic atom energy.

3.3 The structure of the output information

The output information is defined in a Kinetics Definition File by two lists: '*POPULATION' and '*YIELD'. Their format was described in the section 3.1. Here we shall list possible distributions to be output. These can be the populations of states and the reactions yields. Population of a state is the number of muons in this state at certain moment of time. Starting time is the time of muon stop in the media. The following population distributions can be requested (the example figures correspond to the Test Run with the Kinetic Definition File C:\Mucat \Run \test \Hot.kin):

1) Time distribution in the energy interval [Emin,Emax], see Fig.5 for example:

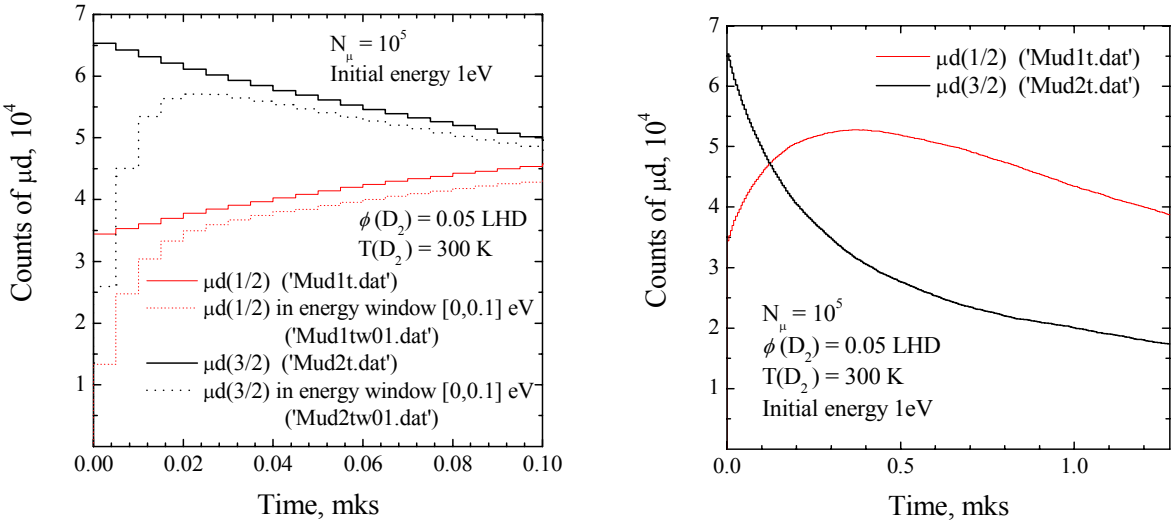


Fig.5. Time distribution of dμ-population.

2) Kinetic energy distribution at certain moment t = Tview, see Fig.6:

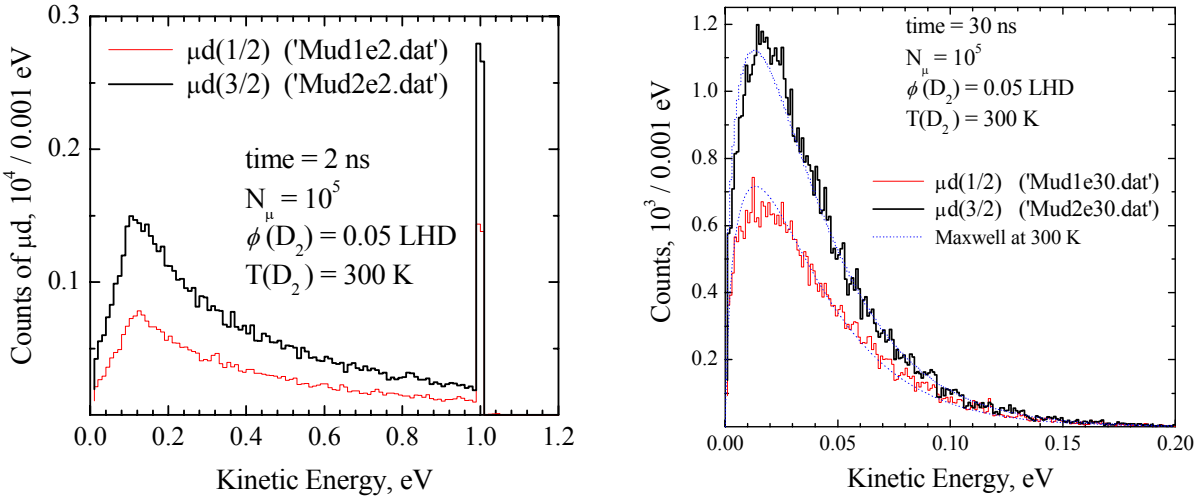


Fig.6. Energy distribution of pμ-atoms.

The reaction yield means the number of transitions of the muon into certain state; besides the final state, the initial state and the transition channel may be specified. If the initial state or the transition channel is not specified, then all possible states and channels are included, according to the kinetic scheme. The following reaction yield distributions can be requested:

1) Time distribution in the specified energy interval [Emin,Emax], an example is shown in the Fig.7:

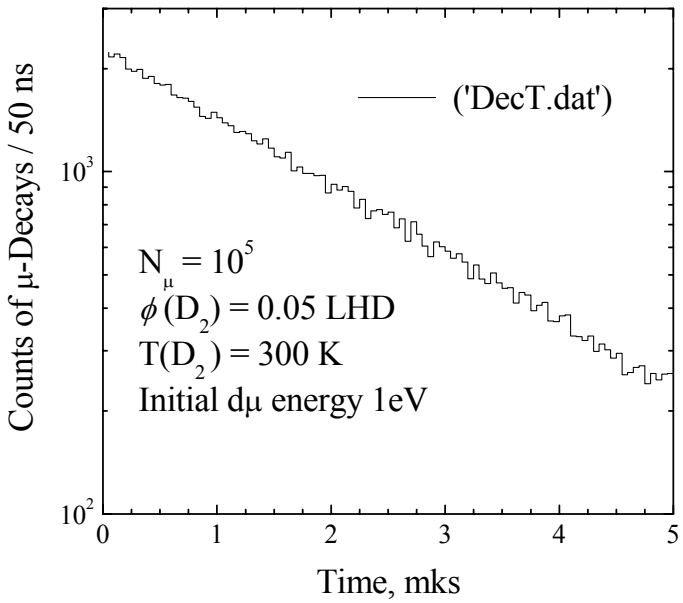


Fig.7. Time distribution of μ-decays.

2) distributions of energies (Fig.8), velocities, distances to the muon stop point (the Range, see the Fig.9), coordinates (X, Y or Z) and of Cos(θ) in the interval [Tmin, Tmax], where θ is the scattering angle in the laboratory system of coordinate and all the kinematic variables correspond to the initial state of the transition. For the latter distributions one can set both time and energy windows, [Tmin, Tmax] and [Emin, Emax]:

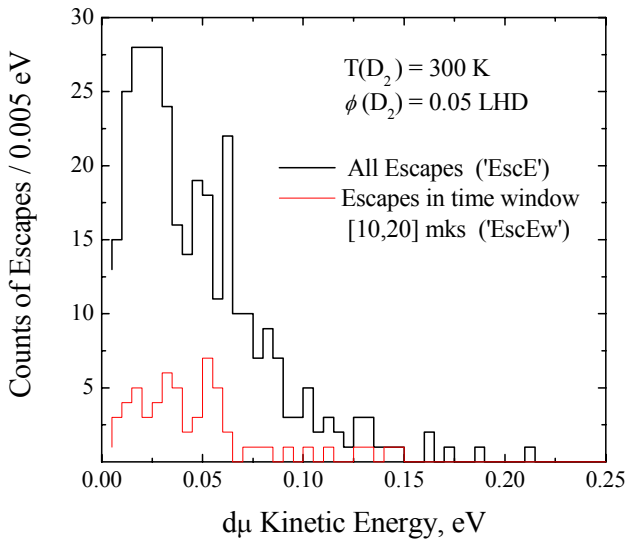


Fig.8. Kinetic Energy distribution of dμ-atoms that escape the target.

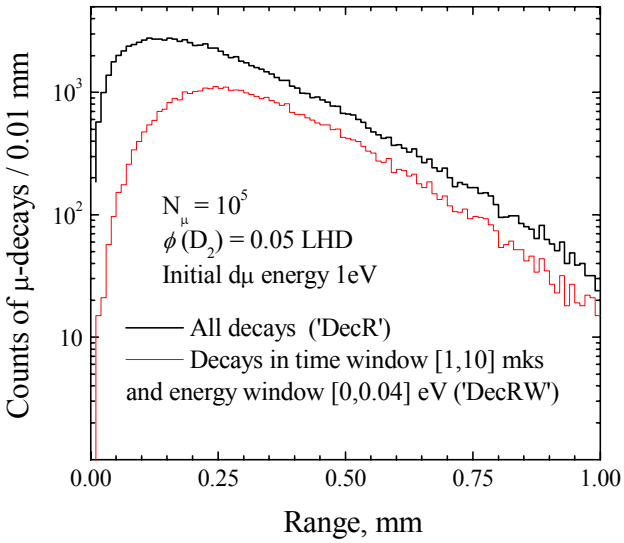


Fig.9. Range distribution of μ Decays in time window [1, 10]mks and dμ-energy window [0.,0.04]eV

All the distributions are output into separate files, in two columns. The first column is the variable, the second – the numbers of counts. Zeroes are replaced by 1.E-04 for appropriate drawing of the graphs in logarithmic scale. The file names are listed in '*POPULATION' and '*YIELD' with extention *.dat. For example, the file DecR.DAT looks like

```
1.00000E-02   185.00
2.00000E-02   574.00
3.00000E-02   996.00
4.00000E-02   1374.0
5.00000E-02   1778.0
  .....         .....
```

Moreover, the Summary Result File is created, with the name given after the Kinetic Definition File with the extension *.sum. It contains some logging information of the run plus the following integral data:

1) The total yield of every state, defined in the kinetic scheme, i.e. how many times the muon has visited these states, divided by the total number of muon series. The total yields of separate states provide easy derivation of the integral parameters of μCF, such as total energy yield. Below you can see the fraction of the file C:\Mucat \Run \test \Hot \Hot.SUM, obtained by running with the kinetic file 'Hot.kin (see section 3.1).

```
============
Total yields
============
 DECAY      0.99660     +-  3.15690E-03
 mu         0.0000      +-  0.0000
 mud1       2.7425      +-  5.23689E-03
 mud2       2.7509      +-  5.24489E-03
 ESCAPE     3.37000E-03 +-  1.83576E-04
====================
```

The Total Yields in this example has the following meaning. During 10^5 muon series, the muon has been in the state 'DECAY' (has decayed) **99660** times. The total yield of 'DECAY' approaches 1 when the maximum muon series time (set at the '*TIME' list) tends to infinity and the yield of '**ESCAPE**' tends to zero. The latter depends on size of the target. Transitions to the state **'mu'** are absent (initialization is not considered to be a transition), so the yield of this state is 0. A muon gets into the state **'mud1'** from any other state **274250** times during 10^5 muon series of cycles. That is only slightly lower than the yield of **'mud2'**.

2) For every requested distribution, the total yield inside of the given distribution boundaries is output. This is the fraction of the total number of events within the requested interval over the number of muon series. Also the mean and the mean square of the distributed variable are printed. For example,

```
============
 Transitions
============
 DecR                Range     0.994      0.265      0.320
   | = file name.dat          |          |          | =<R>    |=√R²
                              |          |= total yield within given interval (and cuts, if any)
                              | = R-distribution
============
```

It should be noted, that during one μCF cycle a muon can visit certain states several times. In general, during one muon series (during lifetime) a muon undergoes several cycles, so the total yield of some states may be greater than 1. The total yield of a distribution also may be greater than 1.

4. Target Geometry

The target is considered to be infinite and homogeneous by default. As it was noted above, the user can define it to be a cylinder, consisting of layers with different contents. The cylinder axis is directed along the muon beam.

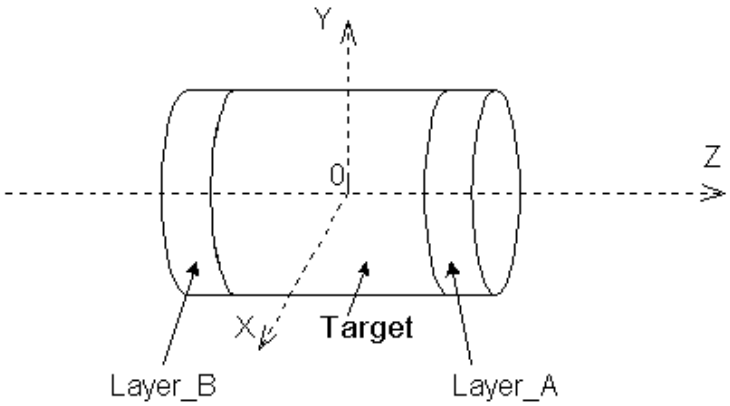


Fig.10. An example of Geometry.

Consider an example of a solid state target, consisting of the main layer 'Target' 0.3 mm thick, between two thin layers 'Layer_A' and 'Layer_B', both 3 mkm thick. Let the main layer consists of hydrogen with a small admixture of tritium and two others — of solid D_2. To introduce such a target geometry into the calculations one has to set the following lists in the Kinetic Definition file:

The list of parameters:

'*PARAMETER'

'CP'	protium density in the target
'CT'	tritium density in the target
'CD2'	Density of molecular deuterium in the layers A and B
'Z1'	Limits of the target along Z axis
'Z2'	
'ZA1'	Limits of the layer A along Z axis
'ZA2'	
'ZB1'	Limits of the layer B along Z axis
'ZB2'	

```
'Zmin'    The limits of muon stop area in the target
'Zmax'
'END'
```

The list of media (various mixtures, vacuum, etc.):

```
'*MEDIA'
    'HTSolid'
    'D2Solid'
    'END'
```

The list of target constituent parts (list of volumes):

```
'*VOLUME'
    'Target'   'HTSolid'  'Z1'  'Z2'
    'Layer_A'  'D2Solid'  'ZA1' 'ZA2'
    'Layer_B'  'D2Solid'  'ZB2' 'ZB1'
    'END'      'END'      ' '  ' '  '
```

This list has the following format:

```
'name'    'media '   'Zmin' 'Zmax'
```

The original idea was to define different parameter sets for different media, and then to define the target parts via the medium name and space limits. In the current version of the program, parameters are defined separately for every volume of the target.

The list of global parameters in the volumes:

```
'*LET'
    'CP'   1.2
    'CT'   1.2E-3
    'CD2'  1.2
    'Zmin'   -.1
    'Zmax'   0.1
    'Z1'     -.15   Geometry of volume 'Target'
    'Z2'     0.15     Thickness = (2*0.15)*(1.2*7.08) = 2.54 mg/cm2
    'ZA1'    0.15   Geometry of volume 'Layer_A'
    'ZA2'    0.153    .003 mm (D2 at 1.2 LHD) <--> 58 mkg/cm2
    'ZB1'    -.15   Geometry of volume 'Layer_B'
    'ZB2'    -.153
    'END' 0.
```

The list defining the media of the target parts:

```
'*LOCAL'
    'Target'      contains only hydrogen with little tritium:
      'CP'   1.2
      'CT'   1.2E-3
      'CD2'  0.
      'END'  0.
    'Layer_A'       consists of solid D2
      'CP'   0.
      'CD2'  1.2
      'CT'   0.
      'END'  0.
    'Layer_B'       consists of solid D2
      'CP'   0.
      'CD2'  1.2
      'CT'   0.
      'END'  0.
    'END'
```

The cylinder radius may be set after the list '*LET':

```
'*RADIUS'
          10.      —  The cylinder radius in mm.
```

After simulation of every transition, the program calculates the azimuthal scattering angle φ and the polar angle θ. So it is possible to extend the program also to 3-dimensional-geometry of media.

It should be noted, that in the "Hot media" model the scattering angles φ and θ are calculated only in case if there are lists '*RADIUS' or '*VOLUME' in the Kinetic Definition File. This trick can accelerate calculations when geometry is not important.

5. The "Hot media" model

To calculate a reaction rate and kinematics variables of a μ-state after a reaction with a molecule of the media, it is necessary to make some assumptions about the motion of media particles. In practice, it has to be done for scattering reactions only, such as elastic and inelastic scattering and spin-flip. All of these reactions are described by the classes '2->2' of the cross-section library.

The "Cold media" model represents the simplest way to do this. It considers the molecule of the medium being at rest prior to any reaction.

So the mesic atom is decelerated in every elastic scattering on a media particle. In this model it keeps 'cooling down' to zero energy, though in reality it will be thermalize after 5 – 6 collisions. In the current version of the program, the energy of a muonic atom is set to Emin (constant) as soon as it becomes below Emin.

To take into account the movement of media molecules in the right way, let us take two colliding particles: a mesic atom a with velocity $\vec{V}_a$ in LAB system and a media particle b. Let there be many sorts of media particles (H_2 or D_2, for example), but we need to consider the only one reaction

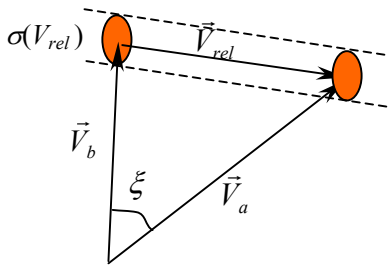
$$a + b \to a' + b',$$

where a' and b' are the mesic atom and the media particles after the scattering, respectively.

The probability density of a particle taken at random to have its velocity equal to V_b and the angle between the vectors $\vec{V}_a$ and $\vec{V}_b$ to be ξ is the Maxwellian one:

$$f_M(V_b, \cos\xi) = f_M(V_b)\, f_M(\cos\xi),$$

where $f_M(V_b)$ is the Maxwellian distribution of absolute velocities, and $f_M(\cos\xi) = \frac{1}{2}$ corresponds to isotropic distribution.



The layout of vectors efore a collision in the "LAB" system.

All theese particles have their velocity $\vec{V}_{rel}$ relative to the atom a. Hence the cross section of such a collision is equal to $\sigma(V_{rel})$ and it is the same for all media particles from that group. The number of particles of this group (with velocity $\vec{V}_b$ and angle ξ) that collide with the mesic atom during a unit-time interval is

$$\sigma(V_{rel})\vec{V}_{rel},$$

normalized to the unit density of particles of one sort. The total number of colliding particles of that sort is

$$\iint V_{rel}\sigma(V_{rel})f_M(V_b)f_M(\cos\xi)dV_b d\cos\xi .$$

And this is actually the rate of the reaction $\lambda(E_a)$.

Thus, for the mesic atom (with velocity V_a) the probability of a collision with the media particle (with velocity V_b) at the angle ξ is:

$$f(V_b,\cos\xi)dV_b d\cos\xi = \frac{V_{rel}\sigma(V_{rel})f_M(V_b)f_M(\cos\xi)dV_b d\cos\xi}{\iint V_{rel}\sigma(V_{rel})f_M(V_b)f_M(\cos\xi)dV_b d\cos\xi}$$

The probability density of a collision of a mesic atom that has kinetic energy E_a with a molecule that has kinetic energy E_b at the collision angle ξ is:

$$\boldsymbol{f(E_b, \cos\,\xi)} = \tfrac{1}{2} f_M(E_b)\frac{\lambda(E_{coll})}{\lambda(E_a)},$$

with the following notations:

$f_M(E_b)$ — Maxwellian energy distribution,

E_{coll} — collision energy, that depends on E_a, E_b and ξ,

$\lambda(E_{coll}) = N_0\ \sigma(E_{coll})\ V_{rel}$,

$N_0 = 4.22 \cdot 10^{22}\ \mathrm{cm}^{-3}$ — the liquid hydrogen density (LHD),

$\sigma(E_{coll})$ — the reaction cross-section in the center of mass system (CMS),

$\lambda(E_a)$ — the reaction rate, averaged over media motion:

$$\lambda(E_a) = \tfrac{1}{2}\int_0^\infty f_M(E_b)\left\{\int_{-1}^{+1}\lambda(E_{coll})\,d\cos\xi\right\}dE_b . \qquad (*)$$

It is possible to simulate the initial energy E_b and the impact angle ξ in LAB using the derived distribution $f(E_b, \cos\xi)$ and two random numbers γ_1 and γ_2. Solving the first equation

$$\int_0^{E_b}\int_{-1}^{1} f(E,x)dE\,dx = \gamma_1 ,$$

we could obtain E_b. The second equation gives us the value $\cos\xi$:

$$\int_{-1}^{\cos\xi} f(E_b,x)dx = \gamma_2 \int_{-1}^{1} f(E_b,x)dx .$$

An advantage of this method is that the code would uses the cross sections of the scattering processes given in CMS, these are taken directly from theoretical calculations. A disadvantage is that this way of simulation of processes can considerably slow down Monte-Carlo calculations because of two reasons. The first one is the additional manipulation: for every scattering event, the code has to calculate the kinematic variables of the mesic atom in CMS, then to simulate them after the scattering in CMS and only then in the LAB system. The second reason is the existence of many channels of reactions (after a scattering the target particle b may land into different excited states b', b'' and so on). Every channel has to be described in a separate *.fcn file of cross sections.

To accelerate the calculations, one needs the integrated characteristics in LAB: the reaction rates in the LAB system $\langle\lambda(\mathrm{E_{lab}})\rangle \equiv \lambda(E_a)$ and the energy-angular distribution in LAB $\langle \mathrm{d}^2\sigma(\mathrm{E_{lab}})/\mathrm{dE_{lab}d}\xi'\rangle$, where $\mathrm{E_{lab}} \equiv E_a$, ξ' is the scattering angle in the LAB system and the angle brackets $\langle..\rangle$ mean averaging over kinematic variables of media molecules at certain temperature.

$$\langle\lambda_n(\mathrm{E_{lab}})\rangle \equiv \lambda_n(E_a) = \tfrac{1}{2}\iint f_M(E_b)\,\lambda_n(E_{coll})\,d\cos\xi\ \ dE_b ,$$

and the double differential cross sections in LAB are calculated in the following way:

$$\langle d^2\sigma_n(\mathrm{E_{lab}})/d\,\mathrm{E_{lab}}\,d\xi\rangle \equiv$$

$$= \left\langle \frac{d^2\sigma_n(E_a)}{dE'_a d\xi'} \right\rangle = \frac{d^2}{dE'_a d\xi'} \iiint f(E_b, \cos\xi) \frac{d\sigma_n(E_{coll})}{d\Omega} d\Omega\, d\cos\xi\, dE_b$$

The kinematic variables in the LAB system after scattering are marked by primes; Ω is the solid scattering angle in CMS. The index n indicates the scattering channels.

It is possible to sum all the channels:

$\langle\lambda(\mathrm{E_{lab}})\rangle = \sum_n \langle\lambda_n(\mathrm{E_{lab}})\rangle$, $\langle d^2\sigma(\mathrm{E_{lab}})/d\,\mathrm{E_{lab}}\,d\xi\rangle = \sum_n \langle d^2\sigma_n(\mathrm{E_{lab}})/d\,\mathrm{E_{lab}}\,d\xi\rangle$

and to deal with only one channel.

5.1 Calculation of rates and double differential cross-sections (CMS —> LAB)

In practice, the code calculates the following values for the single channel only: $\langle\lambda_n(\mathrm{E_{lab}})\rangle$ and

$$\langle d^2\sigma_n(E_{lab})/dE_{lab}\,d\xi'\rangle \equiv$$

$$\frac{\Delta\sigma_n(E_a)}{\Delta E'_a \Delta\xi'} = \frac{1}{2\Delta E'_a \Delta\xi'} \int_0^\infty f_M(E_b) \left\{ \int_{-1}^{+1} \frac{\lambda_n(E_{coll})}{\lambda_n(E_a)} \left[\int \frac{d\sigma_n(E_{coll})}{d\Omega} d\Omega \right] d\cos\xi \right\} dE_b$$

In this expression integration over Ω runs in such a way that the mesic-atom energy and the scattering angle stay within the fixed intervals $[E'_a; E'_a + \Delta E'_a]$ and $[\xi'; \xi' + \Delta\xi']$.

In the code another scheme is realized. The cycles run over all the variables: $\cos\theta$, α, ($d\Omega = d\cos\theta\, d\alpha$), $\cos\xi$, E_b for every E_a. For every set of these variables the final energy E'_a and the scattering angle ξ' in LAB system are calculated and the corresponding bin $[d\sigma(E_a, E'_a, \xi')]$ is incremented by the value

$$\frac{1}{2\Delta E'_a} f_M(E_b) \frac{\lambda(E_{coll})}{\lambda(E_a)} \frac{d\sigma(E_{coll})}{d\Omega} \Delta\cos\theta\, \Delta\alpha\, \Delta\cos\xi\, \Delta E_b\,. \qquad (**)$$

(The index n of the channel number is omitted here and further on). This corresponds to the double differential cross section integrated over the scattering angle within the angle bin:

$$\int_{\xi'}^{\xi'+\Delta\xi'} \frac{d^2\sigma(E_a)}{dE'_a d\xi'} \approx \frac{\Delta\sigma(E_a)}{\Delta E'_a \Delta\xi'} \Delta\xi'\,.$$

The 101-point logarithmic grid for energy values is given in the file \Grids\ENERG101.txt. The cycles over E_a, E'_a and E_b run really on this grid. All calculations in the "Hot media" model go with this tolerance interval on kinetic energy.

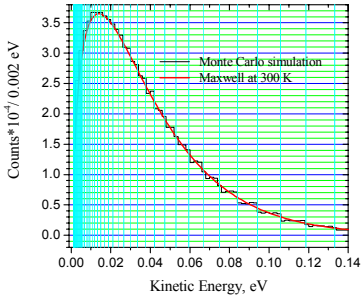


Fig. The energy distribution of mesic atoms in the model with constant scattering cross section. The vertical lines in this figure correspond to the left edges of the intervals of the energy grid.

The grids for $\cos\xi$ and $\cos\theta$ in these calculations are given in \Grids\Angle.cms. The cycle over α runs with constant step AlphaBin=$2\pi/40$ that is defined in the included file \fort\scr10\IntegrPa.inc of the project. The step over ξ' is the same as in *.trm files (see 5.3).

To calculate the contributions (**) into the differential cross section in the LAB system $d\sigma(E_a,\ E'_a,\xi')$ the code must be able to obtain the values $E_{coll} = E_{coll}(E_a, E_b, \cos\xi)$, $E'_a = E'_a(E_a, E_b, \cos\xi, \alpha, \cos\theta)$ and $\xi' = \xi'(E_a, E_b, \cos\xi, \alpha, \cos\theta)$.

Let m_a, m_b, m'_a, m'_b be the masses of particles of the reaction

$$a + b \to a' + b'$$

respectively and the total mass M is

$$M = m_a + m_b = m'_a + m'_b .$$

Then the collision energy equals to

$$E_{coll} = \frac{m_a m_b}{2M} V_{rel}^2, \quad where\ V_{rel} = \sqrt{V_a^2 + V_b^2 - 2V_a V_b \cos\xi}.$$

This is actually $E_{coll}(E_a, E_b, \cos\xi)$, taking into account that $V_a = \sqrt{\frac{2E_a}{m_a}}$ and $V_b = \sqrt{\frac{2E_b}{m_b}}$.

The collision energy corresponds to the initial energy of two particles in CMS:

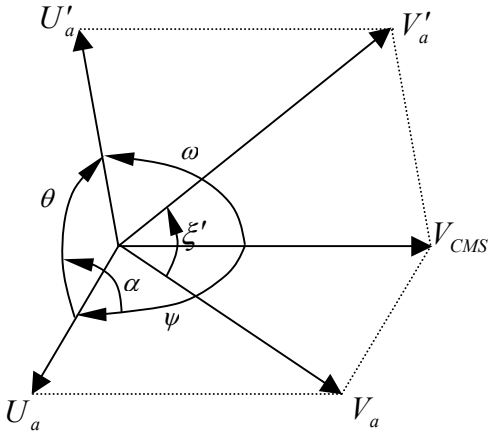
$$E_{coll} \equiv E_{iCMS}.$$

Then the final energy E_{fCMS} after the reaction in CMS is equal to:

$$E_{fCMS} = E_{iCMS} + \Delta E_{if},$$

where ΔE_{if} is given in *.fcn file.

The following figure shows the introduced angles:



V_{CMS} is the velocity of the center of mass in LAB system, U_a and U'_a — velocities of the mesic atom a in CMS before and after the scattering respectively.

$\vec{V}_a = \vec{V}_{CMS} + \vec{U}_a$; $\quad \vec{V}'_a = \vec{V}_{CMS} + \vec{U}'_a$.

Then

$$E'_a = \frac{m'_a V'^2_a}{2} = \frac{m'_a}{2}[V^2_{CMS} + V'^2_a + 2V_{CMS} V'_a \cos\omega], \text{ and}$$

$$\cos\xi' = \frac{\vec{V}_a \vec{V}'_a}{V_a V'_a} = \frac{V^2_{CMS} + V_{CMS} U'_a \cos\omega + U_a U'_a \cos\theta + V_{CMS} U_a \cos\psi}{V_a V'_a},$$

where $\cos\omega = \cos\psi\cos\theta + \sin\psi\sin\theta\cos\alpha$.

These are the derived expressions $E'_a = E'_a(E_a, E_b, \cos\xi, \alpha, \cos\theta)$ and $\xi' = \xi'(E_a, E_b, \cos\xi, \alpha, \cos\theta)$, taking into account the following exrelations:

$$U_a = V_{rel}\frac{m_b}{M}; \quad U'_a = \sqrt{\frac{2E_{fCMS}}{M}\frac{m'_b}{m'_a}}; \quad V_{CMS} = \frac{\sqrt{2}}{M}\sqrt{m_a E_a + m_b E_b + V_a V_b \cos\xi};$$

$$\cos\psi = \frac{\vec{U}'_a \vec{V}_{CMS}}{U'_a V_{CMS}} = \frac{2(E_a - E_b) + (m_b - m_a)V_a V_b \cos\xi}{M V_{rel} V_{CMS}}.$$

There may be several uncertainties. They are resolved as follows:

if $V_a = 0$ or $V'_a = 0$, then $\cos\xi'$ is set to be equal to $\cos\theta$,

if $V_{CMS} = 0$ then the following settings are performed: $E'_a = E_{fCMS} m'_b / M$ and $\cos\xi' = \cos\theta$,

if $V_{rel} = 0$ then $\cos\omega$ is set to be equal to $\cos\theta$.

The result of summation of all the contributions (**) to the double differential cross-section is accumulated firstin the array "DoubDiff"(E_a, E'_a, ξ'). There are maximum elements MaxDD(E_a) of the array for every E_a-bin. To save the computer memory, only those only elements are output into *.trm file that exceed the value MaxDD(E_a)*10^{-4}:

$$\text{DoubDiff}(E_a, E'_a, \xi') / \text{MaxDD}(E_a) \geq \text{eps2},$$

where eps2 = 10^{-4} is set in the"IntegrPa.inc" include file.

Calculation of the double differential cross-section (**) is accompanied with obtaining the reaction rate (*). For every E_a and E_b from the energy grid the following integral is calculated by the function GAUSS of the CERN library:

$$G(E_a,E_b) = \int_{-1}^{+1} \lambda(E_{coll})\, d\cos\xi \ .$$

Then summation over all grid points i of E_b is performed:

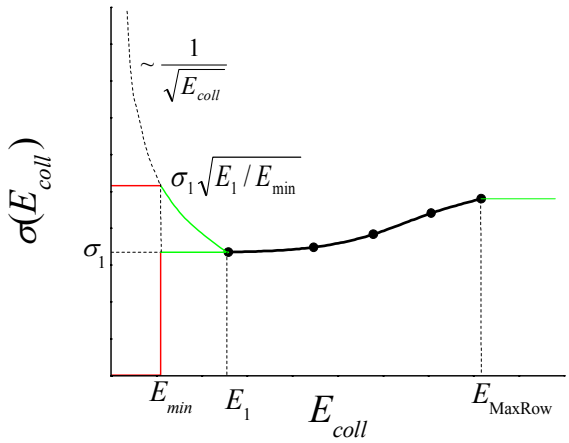
$$\lambda(E_a) = \sum_b f_M(E_b^i) G(E_a, E_b^i) \Delta E_b^i,$$

where E_b^i and ΔE_b^i are the value in the middle point and the width of *i*-th energy bin, respectively.

Calculations of rates and double differential cross-sections (CMS —> LAB) are performed by the subroutine "CMSLab" from the file Jeitler3.for of the project. This subroutine is called from the subroutine "KFCN22". The final kinematic variables $E'_a(E_a, E_b, \cos\xi, \alpha, \cos\theta)$ and $\xi'(E_a, E_b, \cos\xi, \alpha, \cos\theta)$ are obtained by the Subroutine "FinLabVar":

$$\frac{d\sigma}{d\Omega} = \frac{\sigma(E_{coll})}{2\pi} \sum_{n=1}^{N} C_n(E_{coll}) \cos^{n-1}\theta,$$

where the total cross section σ and coefficients C_n are given in *.fcn file in several energy points, and $\sigma(E_{coll})$ is calculated by the Function "Sigma(Ecoll)".



This figure illustrates interpolation and extrapolation of the total cross section. There are *MaxRow* points (black circles) given in *.fcn file. Spline interpolation is implemented inside of

the range $E_{coll} \in [E_1;E_{MaxRow}]$. For $E_{coll} > E_{MaxRow}$ the cross section is assumed to be constant: $\sigma(E_{coll}) = \sigma(E_{MaxRow})$. For elastic scattering (when $\Delta E_{if} = 0$) there is a cut to zero below E_{min} (even if $E_{min}>E_1$) and the cross section is constant $\sigma(E_{coll}) = \sigma(E_1)$ for $E_{coll} \in [E_{min};E_1]$. For inelastic scattering the constant values of the cross section are set $\sigma(E_{coll}) = \sigma_1\sqrt{E_1 / E_{\min}}$ below E_{min} and $\sigma(E_{coll}) = \sigma_1\sqrt{E_1 / E_{coll}}$ for $E_{coll} \in [E_{min};E_1]$.

Thus for precise CMS—>LAB calculations it is necessary to have $E_1 << kT$, where k is Bolzman's constant and T stands for the media temperature. For a reference, $T=300K$ corresponds to $kT \sim 0.04\,\text{eV}$.

Calculation of the Maxwell distribution

$f_M(E_b) = 2\pi(\pi kT)^{-3/2}\sqrt{E_b}\,e^{-E_b/kT}$

is done by the Function "Maxwell"(E_b). It is set to zero at large energies, not to deal with very small numbers:

$$\text{Maxwell}(E_b) \equiv 0, \text{ when } E_b / kT > 50.$$

5.2 Simulations with the "Hot media" model

The problem is to to obtain the kinetic energy and the direction of motion of a mesic particle after its scattering on a media particle. The Subroutine "KFCN22(L,Mode)" with Mode=2 performs this operation, with the initial energy E_a and the direction of motion given.

First of all, the code calculates the energy bin IE_a that corresponds to the energy E_a. (The Subroutine "FindBin" makes this. Searching for IE_a starts from the number determined in the previous scattering.) Then the energy bin IE'_a of the mesic atom after the scattering is found as the upper limit of the sum:

$$\sum_{IE=1}^{IE'_a}\frac{d\sigma}{dE'_a}(IE_a, IE)\Delta IE < \gamma\sigma^{total}(IE_a) < \sum_{IE=1}^{IE'_a+1}\frac{d\sigma}{dE'_a}(IE_a, IE)\Delta IE,$$

where $\gamma \in [0;1]$ is a random number; $\Delta IE = \Delta E(IE)$ is the width of the bin; IE stands for the bin number corresponding to the scattering energy; $\sigma^{total}(IE_a) = \sum_{IE'_a}\frac{d\sigma}{dE'_a}(IE_a, IE'_a)\Delta E'_a$ is the total cross section, and $\frac{d\sigma}{dE'_a}(IE_a, IE'_a) = \sum_{I\xi'}\frac{d^2\sigma\,\Delta\xi'}{dE'_a d\xi'}(IE_a, IE'_a, I\xi')$ is the energy distribution of scattered mesic atoms. The summation on scattering angle bins $I\xi'$ runs over all available bins for given values of IE_a and IE'_a.

The total σ^{total} and differential cross sections $\frac{d\sigma}{dE'_a}(IE_a, IE'_a)$ are stored during the reading of the structure $\frac{d^2\sigma\,\Delta\xi'}{dE'_a d\xi'}$ from *.trm file (by the Subroutine "ReadStr" from the file "Thermal.for").

Finally, the energy of the mesic atom after scattering is obtained as follows:

$$E'_a = E'_a(IE'_a) + \gamma\,\Delta E'_a(IE'_a).$$

So, in the "Hot media" model the kinetic energy is constant inside of every energy bin.

If the calculation of muon coordinates is required (the geometry flag is set: "FlGeom =.true."), then the scattering angle bin number $I\xi'$ is obtained in the same way as IE'_a, with the same Subroutine "ThermKin" from the file Thermal.for:

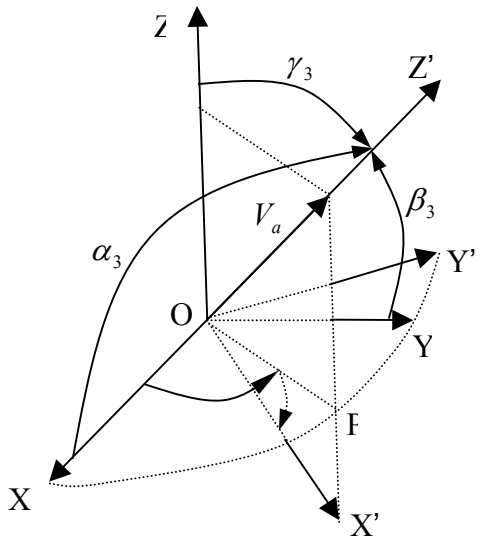
$$\sum_{I\xi=1}^{I\xi'} \frac{d^2\sigma\ \Delta\xi'}{dE'_a d\xi'}(IE_a, IE'_a, I\xi) < \gamma \frac{d\sigma}{dE'_a}(IE_a, IE'_a) < \sum_{I\xi=1}^{I\xi'+1} \frac{d^2\sigma\ \Delta\xi'}{dE'_a d\xi'}(IE_a, IE'_a, I\xi).$$

And the scattering angle is

$$\xi' = \xi'(I\xi') + \gamma\ \Delta\xi'(I\xi'),$$

where $\Delta\xi'(I\xi')$ is the width of the angular bin.

The direction of motion after scattering is obtained in the following way.



Let {X,Y,Z} be the original coordinate system, in which the axis OZ is along the muon beam direction. Then the velocity $\vec{V}_a$ has the following projections:

$$\frac{\vec{V}_a}{V_a} \begin{cases} \text{X}: & \cos\alpha_3 \\ \text{Y}: & \cos\beta_3 \\ \text{Z}: & \cos\gamma_3 \end{cases}$$

Besides, another coordinate system {X',Y',Z'} is associated with $\vec{V}_a$. The angles between the axes of these coordinate systems may be briefly expressed by the diagram

	X	Y	Z
X'	α_1	α_2	α_3
Y'	β_1	β_2	β_3
Z'	γ_1	γ_2	γ_3

One coordinate system {X,Y,Z} may be transformed to the other {X',Y',Z'} by two rotations. The first rotation is around the axis OZ until OX is aligned with OP, which is the projection of OZ' onto the plane XOY. The second rotation is around the axis OY' until OZ is aligned with OZ'. For such orientation of {X',Y',Z'} with respect to {X,Y,Z}, the following expressions are valid:

$$\cos\alpha_1 = \cos\gamma_3 \cos\beta_2; \qquad \cos\alpha_2 = -\cos\beta_3 / \sin\gamma_3;$$
$$\cos\beta_1 = -\cos\gamma_3 \cos\alpha_2; \qquad \cos\beta_2 = \cos\alpha_3 / \sin\gamma_3;$$
$$\cos\gamma_1 = -\sin\gamma_3; \qquad \cos\gamma_2 = 0.$$

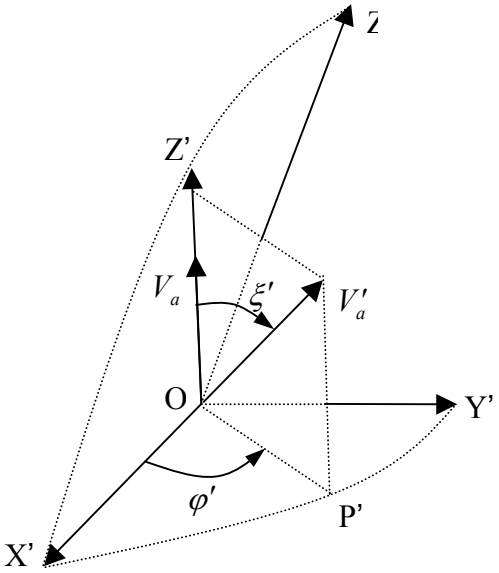
And the original coordinates expressed in terms of the primed ones are

$$\text{X} = \text{X}'\cos\alpha_1 + \text{Y}'\cos\alpha_2 + \text{Z}'\cos\alpha_3;$$
$$\text{Y} = \text{X}'\cos\beta_1 + \text{Y}'\cos\beta_2 + \text{Z}'\cos\beta_3;$$
$$\text{Z} = \text{X}'\cos\gamma_1 + \text{Y}'\cos\gamma_2 + \text{Z}'\cos\gamma_3.$$

The new direction of motion of the mesic atom after scattering is expressed as follows:

$$\frac{\vec{V}'_a}{V'_a} \begin{cases} \mathrm{X}': & \sin\xi'\cos\varphi' \\ \mathrm{Y}': & \sin\xi'\sin\varphi' \\ \mathrm{Z}': & \cos\xi' \end{cases}$$

Here φ' is the polar angle and it is calculated as $\varphi' = 2\pi\gamma$, where γ is a random number, uniformly distributed in [0;1].



Then this direction in terms of the original coordinate system is

$$\frac{\vec{V}'_a}{V'_a} \begin{cases} \mathrm{X}: & \cos\alpha_1 \sin\xi'\cos\varphi' + \cos\alpha_2 \sin\xi'\sin\varphi' + \cos\alpha_3 \cos\xi' \\ \mathrm{Y}: & \cos\beta_1 \sin\xi'\cos\varphi' + \cos\beta_2 \sin\xi'\sin\varphi' + \cos\beta_3 \cos\xi' \\ \mathrm{Z}: & \cos\gamma_1 \sin\xi'\cos\varphi' + \cos\gamma_2 \sin\xi'\sin\varphi' + \cos\gamma_3 \cos\xi' \end{cases}$$

There is the array RV(3,3) in the code (Subroutine "NewDirec" in the file "Thermal.for") that stores the rotation matrix:

$\mathrm{RV}(1,1) = \cos\alpha_1$; $\mathrm{RV}(1,2) = \cos\alpha_2$; $\mathrm{RV}(1,3) = \cos\alpha_3$;

$\mathrm{RV}(2,1) = \cos\beta_1$; $\mathrm{RV}(2,2) = \cos\beta_2$; $\mathrm{RV}(2,3) = \cos\beta_3$;

$\mathrm{RV}(3,1) = \cos\gamma_1$; $\mathrm{RV}(3,2) = \cos\gamma_2$; $\mathrm{RV}(3,3) = \cos\gamma_3$;

So, RV(j,3) is a unit vector of the velocity in LAB. And according to the expressions above, the new (after scattering) array RV' is calculated from the old (before the scattering) as follows:

$$\mathrm{RV'}(1,3) = \mathrm{RV}(1,1)\sin\xi'\cos\varphi' + \mathrm{RV}(1,2)\sin\xi'\sin\varphi' + \mathrm{RV}(1,3)\cos\xi';$$

$$\mathrm{RV'}(2,3) = \mathrm{RV}(2,1)\sin\xi'\cos\varphi' + \mathrm{RV}(2,2)\sin\xi'\sin\varphi' + \mathrm{RV}(2,3)\cos\xi';$$

$$\mathrm{RV'}(3,3) = \mathrm{RV}(3,1)\sin\xi'\cos\varphi' + \mathrm{RV}(3,2)\sin\xi'\sin\varphi' + \mathrm{RV}(3,3)\cos\xi';$$

The other elements are calculated from RV'(j,3):

$\mathrm{RV'}(1,2) = -\mathrm{RV'}(2,3)/\sqrt{1-\mathrm{RV'}(3,3)^2}$; $\mathrm{RV'}(2,2) = \mathrm{RV'}(1,3)/\sqrt{1-\mathrm{RV'}(3,3)^2}$; $\mathrm{RV'}(3,2) = 0$;

$\mathrm{RV'}(1,1) = \mathrm{RV'}(3,3)\,\mathrm{RV'}(2,2)$; $\mathrm{RV'}(2,1) = -\mathrm{RV'}(3,3)\,\mathrm{RV'}(1,2)$; $\mathrm{RV'}(3,1) = -\sqrt{1-\mathrm{RV'}(3,3)^2}$.

Thus having got the scattering angle, the code calculates the new direction of motion after the reaction.

5.3 The format of files with the rates and double differential cross-sections

Summarizing, the code uses the reaction rates in LAB system $\langle\lambda(E_{lab})\rangle$ and the double differential cross sections $\langle d^2\sigma(E_{lab})/d E_{lab} d\xi'\rangle$. The code can construct these data from the cross-sections given in CMS and presented in *.fcn file of '2->2 ' class, if necessary. The data $\langle\lambda(E_{lab})\rangle$ and $\langle d^2\sigma(E_{lab})/d E_{lab} d\xi'\rangle$ are stored in files *.tra and *.trm respectively. The names of these files are the same as for *.fcn and are indicated in the list '*LINK' of the Kinetic Definition File. All these three files must be put into one FCN\fcn_n directory (see the section "Installation of MUCAT code on a computer"). For example:

'C:\Mucat\fcn\fcn_4\dd11.fcn' cross-sections and angular distributions in CMS
'C:\Mucat\fcn\fcn_4\dd11.tra' the reaction rates in LAB
'C:\Mucat\fcn\fcn_4\dd11.trm' double differential cross sections in LAB

It is important for this purpose that *.fcn file must be of '2->2 ' class, which is processed by the SUBROUTINE KFCN22. Only this class can deal with "Hot media" model. If both *.tra and *.trm files are given and the "Cold media" model is not implemented, then the *.fcn file may be reduced to its first three lines (besides, only 'M3' in the third line is needed). Otherwise it is used in its whole volume.

The data in *.tra and *.trm files strongly depend on the Target (media) Temperature, which value stands in the first line of these files (see the section 5.1). If the *.trm file, corresponding to the first scattering process in the Kinetic Definition file, exists, then the temperature is taken from it. Otherwise, it is prompted from the console (see the Test Running section). The media temperature is set once per run. The coincidence of the temperature values is checked for all *.trm and *.tra files involved and warnings appear if they are not the same (see the Test Running), but it does not influence on the run.

When the user has got *.tra or both *.tra and *.trm files for some temperature and needs to rebuild them for another temperature value, he has to delete them or rename, then MUCAT code builds them anew as needed. During creation of a *.trm file, the corresponding *.tra file is created mandatory.

Strictly speaking, all the files *.fcn, *.trm and *.tra should be built or taken for the same media temperature. (Though the *.fcn files contain data in CMS, they may depend on the temperature due to averaging over rotational levels of target molecules). But the code allows using of any available data.

The reaction rates $\langle\lambda(E_{lab})\rangle$, as well as the double differential cross sections $\langle d^2\sigma(E_{lab})/d E_{lab} d\xi'\rangle$, are created directly from corresponding differential cross sections in CMS: $d\sigma(E_{coll})/d\Omega$. It is not quite correct to obtain $\langle\lambda(E_{lab})\rangle$ from $\langle d^2\sigma(E_{lab})/d E_{lab} d\xi'\rangle$ due to the inequality

$$\langle\lambda(E_{lab})\rangle = \langle V_{rel}\sigma\rangle \neq V_{rel}\langle\sigma\rangle = \iint V_{rel}\langle d^2\sigma(E_{lab})/d E_{lab} d\xi'\rangle d E_{lab} d\xi'.$$

It can be obtained from so called double differential rates in LAB:

$$\langle\lambda(E_{lab})\rangle = \iint\langle d^2\lambda(E_{lab})/d E_{lab} d\xi'\rangle d E_{lab} d\xi',$$

if they are available.

Note that a *.trm file may contain $\langle d^2\lambda(E_{lab})/d E_{lab} d\xi'\rangle$ or any other magnitude that provide right energy and angular distributions of scattered particles in LAB system. But the usage of differential rates seems to be not quite correct for calculation of kinematic variables after scattering. For this purpose one should use differential cross sections.

A fragment of the *.tra file with $\langle\lambda(E_{lab})\rangle$ ("dd11.tra") is quoted below:

300.0 K Rates, 1/mks via energy, eV in lab.
Energy channels from ENERG101.txt

Grid	InitEn	Rate
1	0.1000E-02	0.1001E+04
2	0.1122E-02	0.1006E+04
3	0.1259E-02	0.1011E+04

…	…	…
99	0.7943E+02	0.6461E+05
100	0.8913E+02	0.6843E+05
101	0.1000E+03	0.7248E+05

The first number corresponds to the target temperature in Kelvins. The rest of this line and other two lines are comments. They say that this file contains reaction rates in units of mks^{-1} (the type of reaction is defined by the file name) versus initial energy of a mesic atom in units of eV. The comments indicate also the name of the file (ENERG101.txt) with the implemented energy grid. The third line is just a header of the table that follows.

The first column ('Grid') corresponds to the number of the energy grid bin, the second ('InitEn') – to the initial energy of the mesic atom (that is the middle value of the energy bin), and the third one ('Rate') is the rate value.

A fragment of the *.trm file with $\langle d^2\sigma(E_{lab})/d E_{lab} d\xi' \rangle$ ("dd11.trm") is quoted below:

300.0 K double diff. x-section in lab. system
Energy channels from ENERG101.txt

InEn	FinEn	Theta	ddSigma
1	1	1	0.1171E-19
1	1	2	0.8278E-20
1	1	3	0.2844E-19
…	…	…	…
101	98	10	0.4737E-21
101	98	11	0.4224E-22
101	99	7	0.4590E-21
101	99	8	0.1332E-20
101	99	9	0.4947E-21
101	99	10	0.1315E-23
101	100	4	0.8519E-23
101	100	5	0.2836E-20
101	100	6	0.1343E-20
101	100	7	0.1120E-20
101	100	8	0.4801E-23
101	101	3	0.1934E-20
101	101	4	0.1642E-20
101	101	5	0.5057E-22

The first three lines are like those in *.tra file; the energy binning is the same. The table contains subsequently: in the first column - the number of initial energy bin ('InEn', corresponding to E_a); in the second column – the number of final energy bin ('FinEn', corresponding to E'_a), in the third column – the number of the scattering angle bin ('Theta', corresponding to ξ')[#], and in the fourth column - the differential cross section (corresponding to $\langle d^2\sigma(E_a)/d E'_a \, d\xi' \rangle$). The linear regular 36-point binning is used for LAB scattering angle ξ' (interval from 0 to 180 degrees). The angular bin with label "1" corresponds to the interval 0--5 deg, etc. In fact, every value in the fourth column is the cross section integrated over the angle within the given angular bin. Therefore, to obtain the total cross section versus initial energy, the code sums the contributions from all angular bins (sums over the third index), WITHOUT cosine factor. However, while summing over final energy, one should MULTIPLY the value from the fourth column by the WIDTH of respective final energy bin.

A fragment of ENERG101.txt file with the 101-point logarithm grid for the energy values is quoted below:

[#] It would be better to call this 'Ksi' instead of 'Theta'.

i	e1(i)	e(i)	e2(i)	de(i)
1	.94250E-03	.10000E-02	.10575E-02	.11500E-03
2	.10575E-02	.11220E-02	.11865E-02	.12903E-03
3	.11865E-02	.12589E-02	.13313E-02	.14478E-03
…	…	…	…	…
99	.74865E+02	.79433E+02	.84000E+02	.91350E+01
100	.84000E+02	.89125E+02	.94250E+02	.10250E+02
101	.94250E+02	.10000E+03	.10575E+03	.11500E+02

The first line is the header and it is ignored by the code. The first column 'i' corresponds to the bin number, the second one 'e1(i)'– to the left edges of bins, 'e(i)'– to middle points of bins, 'e2(i)'– to the right edges of bins and 'de(i)'– to the widths of the bins.

The name of the file that defines the energy grid stands in the included file en_grid.inc:

Parameter (NGrid=101, HenerGr='ENERG101.txt', AngGrid=36)

The parameters 'NGrid' and 'AngGrid' are respectively the total number of energy and angular bins in the *.trm files. All the *.trm and *.tra files must have the same grids.

The 'HenerGr' stands for the file name. The code searches for this file in the directory %BASE%\Grids and in the current directory if %BASE% is not defined.

Appendixes

A. Installation of the MUCAT code on a computer

The full archive (MUCAT.zip), which contains the FORTRAN-code, the Cross-Section Library, several testing examples, documents, cross-section data, some useful tools and the short versions of the code, takes about 19 MB. Unpacked, it takes about 50 MB. The executable file, created after the FORTRAN-project compilation, takes 512 KB. The Test Run requires about 135 MB of RAM in addition to what the OS takes.

To install the program, one has to do the following.

1. **Unpack the file MUCAT.zip into some directory, say, C:\.**

Then the directory C:\MUCAT will be created. We refer to it as %BASE%.

You get the following:

```
C:\MUCAT\                — this is %BASE%
        |\ README.txt     — file with brief instructions
        |\ Data\         — Archive of ZIP and GZ files with cross sections
        |\ Docum\        — Archive of ZIP files with documents, including this manual
        |\ fcn\ fcn_1\          — the kinetics library
        |      \ fnc_2\
        |      \ fnc_3\
        |      \ fnc_4\
        |\ fort\ src10\     — the FORTRAN source code of the current version
|       \ src9\      — the FORTRAN source code of 9 version
|\ Grids\ ENERG101.txt — file with the energy grid
|         \ Angle.cms       — file with the angle grid
|         \ Grids.zip       — Archive of other grids
|\ Project\                  —  Fortran project
   |       |\ Mucat10\Mucat10.dsp  — developer studio project of 10 version
|       |             \ Debug\ Mucat10.exe — Executable file for Win'98
|        \ Mucat9\ Mucat9.dsp  — developer studio project of 9 version
|                    \ Debug\Mucat9.exe — Executable file for Win'98
|\ Run\           — some examples of kinetics
|    |\ dmu_D2\  — Kinetics simulation  for dμ in D2
|    |\ Examles\  — Simulation  for globules and dμ+p
|    |\ test\    — test running for the both versions v.9 and v.10
|     \ Thermal\   — thermalization with double diff. x-section and rates
```

```
|\ Scr\            — scripts  for using various fcn_* and versions 9 or 10.
|\ Tools\          — short tools written on Fortran
|        |\ Addit\         — additional useful tools
|        |\FCN21Creation\   — code for creation of FCN '2->1 0' file
|         \Maxwell\Maxwell.zip — code for creation of Maxwell energy distribution
 \ Versions\ Mucat10.zip      — current version in short form
             \ Mucat9.zip     — previous version in short form
```

2. Make the executable file Mucat10.exe.

There are two executable files already compiled for Windows'98. They are Mucat10.exe and Mucat9.exe that correspond to different versions of the code: 10-th is the current version and 9-th is the previous one with the "Cold media" model only. They are placed in different directories, as one can see in the tree above. The easiest way to create them is to use Mucat*.dsp or *.dsw file of Visual Fortran 6.0.A. If Visual Fotran is not available just compile the following files of the FORTRAN project, resident in %BASE%\ fort\ src10:

Fcnlib1.for	Kfcn22dz.for	Mcprob_a.for
GAUSS.FOR	KFCN22Z_16.for	RND4.FOR
GkFCN_16.for	Kfcna_.for	Thermal.for
ICHKOPEN.FOR	Mccalc_a.for	TIDAVAX.FOR
Kfcn.for	MCGEOM_A.FOR	Jeitler3.for
KFCN12W.FOR	MCGETRES.FOR	
Kfcn21rs.for	Mckmain.for	

Put the executable into %BASE%\ Project\ Mucat10\ Debug\ MUCAT10.exe

3. Run the program

Under DOS or Windows it can be run by a *.bat file from any directory, for example: C:\Mucat\Run\test\runV10.bat (see the Appendix B).

Just change directory to C:\Mucat\Run\test\:

```
>cd C:\Mucat\Run\test
```

and run runV10.bat:

```
>runV10
```

This *.bat file contains the reference to a *.kin file from the same directory and to a script from %BASE% \scr. See the contents of C:\Mucat\Run\test\runV10.bat below:

```
..\..\Scr\MUC_4.bat Hot
Pause
```

This file uses the Hot.kin as a Kinetic Definition file and MUC_4.bat as the script. This script runs Mucat10.exe with fcn_4 as a FCN library that is defined by the number 4 in the file name. The general scheme of internal dependencies is demonstrated in the Figure below.

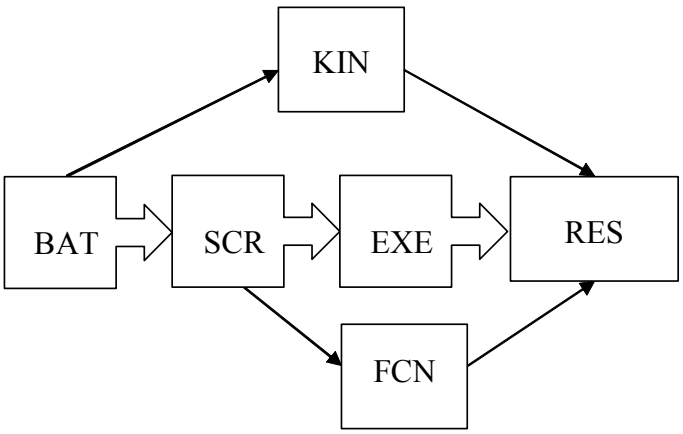


Fig. The block diagram of the code running.
BAT — a starting file (%BASE%\Run\ *\ *.bat),
SCR — a script file (%BASE%\scr\ *.bat),
KIN — Kinetic Definition File (%BASE%\Run\ *\ *.kin),
EXE — the executable file (%BASE%\ Project\ Mucat*\Debug\Mucat*.exe),
RES — the results (%BASE%\Run\ *\ *\ *.dat),,
FCN — the library of cross sections (%BASE%\fcn\ fcn_* *.*),
→ — means what defines what,
⇨ — stands for the main direction of the code execution.

There are several scripts with names MUC_*.bat. They all run the code Mucat10.exe. The scripts with names MCK_*.bat run the old version Mucat9.exe. The number in place of * corresponds to the FCN library %BASE%\fcn\fcn_*\ .

The contents of C:\Mucat\Scr\MUC_4.bat Hot isfollowing:

```
@echo off
rem MUC_4.bat                          March 2002
rem
rem Run the MUCAT10 code with the FCN\fcn_4 library.
rem
rem Usage:
rem     > MUC_4 FileName
rem where FileName.KIN is a kinetics definition file.
rem The results are written to the subdirectory FileName.
rem

:SetEnv
rem --- edit the following 2 lines with "SET" if needed (no trailing spaces!)
rem ********************************************************************
echo on
SET BASE=C:\Mucat
SET FCNLIB=%BASE%\FCN\fcn_4
@echo off
rem ********************************************************************
echo ____________________________________________________________________
echo You may delete "PAUSE" in %BASE%\SCR\MUC_4.bat if "SET" is OK.
echo Increase Evironment memory of the session if 'out of environment space'
rem Delete or comment the following line if set is OK
Pause
rem ------------------------------------------------------------

echo *** Monte Carlo Kinetics *** v.10(thermal) 2002 I.M. ***
echo *** Kinetics definition file: %1.KIN
echo *** The FCN library path: %FCNLIB%

:ChkKin
DIR *.KIN
rem   IF EXIST %1.KIN GOTO Run
rem   echo !!! File %1.KIN not found -- Stop.
```

```
rem   GOTO End

:Run
COPY %1.KIN MCK.KIN
echo running Mucat.exe
%BASE%\Project\MUCAT10\Debug\Mucat10.exe
echo You may delete "PAUSE" in %BASE%\SCR\MUC_4.bat if running is OK.
rem Delete or comment the following line if running is OK
pause

:SaveRes
MKDIR %1
COPY MCK.RES %1\%1.SUM
COPY *.MCK %1\*.DAT
DEL  *.MCK
rem   DIR %1

:End
```

Everyone can easily edit this file changing principally these three most important lines:

```
SET BASE=…
SET FCNLIB=…
%BASE%\Project\MUCAT10\Debug\Mucat10.exe
```

If unpacking into that particular subdirectory %BASE% is not acceptable, then edit the line SET BASE= . . . , setting here the path to some other subdirectory. After creating a new FCN directory, the new path to it should be typed in SET FCNLIB= . . . The third line is the full path to the executable file of the code.

If you are going to use another OS, you have to modify the *.bat file according to it. Under UNIX you can use MUC_1.sh file, located in the same subdirectory %BASE%\scr\.

There are archives of the short versions of Mucat10 and Mucat9 in the subdirectory %BASE%\Versions\. They are independently functional codes with their cross-sections libraries, test examples and usage instructions. Mucat10.zip takes 382 KB that is even less than 399 MB of Mucat9.zip, because Mucat9.zip contains more testing examples in the subdirectory Mucat\run\test.

B. The test run of MUCAT

Change to this directory: C:\Mucat\Run\test\

```
>cd C:\Mucat\Run\test
```

and run runV10.bat:

```
>runV10
```

This *.bat file runs the script C:\Mucat\scr\MUC_4.bat, which uses FCN library C:\Mucat\fcn\fcn_4 and Kinetic definition file C:\Mucat\Run\test\Hot.kin with executable module C:\Mucat\Project\Mucat10\Debug\Mucat10.exe. The Kinetic definition file Hot.kin is quoted in the section 3.1.

You must see the following:

```
------------------------------------------------------------
C:\Mucat\RUN\test>..\..\Scr\MUC_4.bat Hot

C:\Mucat\RUN\test>SET BASE=C:\Mucat

C:\Mucat\RUN\test>SET FCNLIB=C:\Mucat\FCN\fcn_4
_____________________________________________________________
You may delete "PAUSE" in C:\Mucat\SCR\MUC_4.bat if "SET" is OK.
Increase Evironment memory of the session if 'out of environment space'
Press any key . . .
```

```
------------------------------------------------------------
```

This pause is created to be sure that the space is enough to set the environment variables. If you see "out of environment space" after some SET operator, you have to press "Ctrl-C" to terminate the run. Then you have to increase the environment space. You can click with the right button of the mouse on runV10.bat and chose "Properties…". Choose the a bookmark "Memory" and type Environment Space volume. Usually 1280 KB is enough.

There is another way to solve the problem of environment space. Include the following line into the file C:\config.sys:

SHELL=C:\WINDOWS\COMMAND.COM C:\WINDOWS /E:1280 /P

Then you have to reboot Windows, and the all the *.bat files will have proper environment space.

After you press any key, the run is goes on:

```
------------------------------------------------------------
*** Monte Carlo Kinetics *** v.10(thermal) 2002 I.M. ***
*** Kinetics definition file: Hot.KIN
*** The FCN library path: C:\Mucat\FCN\fcn_4

 Volume in drive D is …..
 Volume Serial Number is …..
 Directory of C:\Mucat\RUN\test

COLD     KIN        1 971  07.04.03  13:00 Cold.kin
HOT      KIN        1 959  07.04.03  12:59 Hot.kin
       2 file(s)              3 930 bytes
       0 dir(s)         8 355,56 MB free
      1 file(s) copied
running Mucat.exe
   >>> Number of events =
------------------------------------------------------------
```

Type the number of muons and press <Enter>, e.g.

>>> Number of events = **100000**

If everything was done correctly, you will get the screen like this:

```
------------------------------------------------------------
  *** Open MCK.RES as summary file
     Monte Carlo Kinetics v.10  MIA March-2002
   *** Open MCK.KIN as input file
   *** FCN library from C:\Mucat\FCN\fcn_4

   *TITLE
   Hot.kin
   *SHOW
   *PARAMETER
    1   CD
    2   Zmin
    3   Zmax
    4   Ethermal
    5   Z1
    6   Z2
   List of parameters:
      0
      1       CD
      2       Zmin
      3       Zmax
      4       Ethermal
      5       Z1
      6       Z2
   *LET
    1   CD          0.100
    2   Zmin        1.000E-06
    3   Zmax       -1.000E-06
    4   Ethermal    0.500
    5   Z1         -10.0
    6   Z2          10.0
   *MEDIA
    1   D2Gas
   List of media:
```

```
    0      VACUUM
    1      D2Gas
  *VOLUME
  Target  :  1     5  6
  *STATE
   1   mu
   2   mud1
   3   mud2
   List of states:
    0      DECAY
    1      mu
    2      mud1
    3      mud2
    4      ESCAPE
  *INITIAL
  Initial state: mu          1
  *LINK
  *** Function initialization active ***
  Function        OK :  0 :  0  1
*** Reading file *C:\Mucat\FCN\fcn_4\Mud_e1.FCN *
  PDLIFCN   6 points are used
  Function Mud_e1  OK :  1 : 406  1
   1    1  mu       2  mud1      1  Mud_e1    1.000E+08
*** Reading file *C:\Mucat\FCN\fcn_4\dd11.FCN *
***  34 points used.


  Enter target temperature (K), please. T =
-------------------------------------------------------------
```

Type the temperature and press <Enter>, e.g.

Enter target temperature (K), please. T = **300.**

Then the calculations of the transformation CMS —> LAB start:

```
-------------------------------------------------------------
*** File dd11    .tra creation starts
 *** Opening file *C:\Mucat\FCN\fcn_4\dd11.tra *
 Calculation CMS-->Lab starts

 Energy grid number
          1      of       101
          2      of       101
          3      of       101
         ...     ...      ...
        100      of       101
        101      of       101
*** Opening file *C:\Mucat\FCN\fcn_4\dd11.trm *

 CMS-->Lab performed successfully

 *** Reading file *C:\Mucat\FCN\fcn_4\dd11.trm *
 *** Reading file *C:\Mucat\FCN\fcn_4\dd11.tra *
   Function dd11    OK :  2 : 201  1
    2     2  mud1      2  mud1      2  dd11      1.000E+00
    ...     ...    ...       ...
-------------------------------------------------------------
```

The long calculation of cross sections CMS—>LAB is over, and now dd11.tra and dd11.trm files appear in %BASE%\fcn\fcn_4. If everything is OK they must be identical with the same from the archive %BASE%\fcn\fcn_4\fcn_4.zip. If you start the calculation again, this long part of calculation will not be performed and you will not be prompted for the temperature.

Meanwhile the running is going on:

```
-------------------------------------------------------------
*** Reading file *C:\Mucat\FCN\fcn_4\dd12.FCN *
 ***  34 points used.
*** Reading file *C:\Mucat\FCN\fcn_4\dd12.trm *
*** Reading file *C:\Mucat\FCN\fcn_4\dd12.tra *
  Function dd12    OK :  3 : 201  2
   3     2  mud1      3  mud2      3  dd12      1.000E+00
*** Reading file *C:\Mucat\FCN\fcn_4\dd21.FCN *
***  28 points used.
*** Reading file *C:\Mucat\FCN\fcn_4\dd21.trm *
*** Reading file *C:\Mucat\FCN\fcn_4\dd21.tra *
   Function dd21    OK :  4 : 201  3
```

```
    4     3  mud2       2  mud1       4  dd21      1.000E+00
*** Reading file *C:\Mucat\FCN\fcn_4\dd22.FCN *
***  28 points used.
*** Reading file *C:\Mucat\FCN\fcn_4\dd22.trm *
*** Reading file *C:\Mucat\FCN\fcn_4\dd22.tra *
   Function dd22     OK :   5 : 201   4
    ...      ...     ...        ...
    1     1   2     1       0    1.000E+08
    2     2   2     2       3    1.000E+00
    3     2   3     3       0    1.000E+00
    4     3   2     4       5    1.000E+00
    5     3   3     5       0    1.000E+00
 VOLUMES ----------------
    1: Target         1     5 -1.000E+01   6  1.000E+01      2   3
         Local Parameters:
           None
    2: VACUUM 1       0     0 -1.000E+19   5 -1.000E+01      0   1
         Local Parameters:
           None
    3: VACUUM 2       0     6  1.000E+01   0  1.000E+19      1   0
         Local Parameters:
           None
 POPULATIONS ------------
    1     2       2    mud            2     1.000E-04     0
          0.000E+00   7.000E+00   5.000E-02    0.000E+00   0.000E+00
    2     2       3    mud1           2     1.000E-02     0
          0.000E+00   5.000E+00   5.000E-02    0.000E+00   0.000E+00
    3     2       4    mud2           2     5.000E-02     0
          0.000E+00   0.000E+00   0.000E+00    0.000E+00   0.000E+00
    4     2       0    mudt           1     0.000E+00     0
          0.000E+00   0.000E+00   0.000E+00    0.000E+00   0.000E+00
 YIELDS -----------------
    1     0   4     0       0    EscT           1     0
          0.000E+00   7.000E+00   5.000E-02    0.000E+00   0.000E+00
                                  0.000E+00   0.000E+00
    2     0   0     0       0    DecT           1     0
          0.000E+00   5.000E+00   5.000E-02    0.000E+00   0.000E+00
                                  0.000E+00   0.000E+00
 Number of States         :  4
 Number of Links          :  6
 Number of Parameters     :  6
 Number of Functions      :  5
 Number of Media          :  1
 Number of Volumes        :  3
 Initial state        :  1
 Ncollision_max :   65535
 T_max              :  2.000E+01
 Decay rate         :  4.550E-01

  Scattering angles and coordinates are calculated
Hote media model is implemented for  temperature 300.0K
below lab. kinetic energy  0.50eV
Cold media model is implemented above
   *** Kinetics definition completed
   *** Wait please. Calculating kinetics ...
   |--------------------|
   |.................

------------------------------------------------------------
```

The running dotted line shows the Monte-Carlo progress. When the Monte-Carlo simulation is completed, you see the screen like this:

```
------------------------------------------------------------
   |--------------------|
   |....................|  Done
                                08-APR-03  23:23:17
   Hot.kin
    Number of events =   100000
   ============
   Total yields
   ============
    DECAY       0.99660     +-  3.15690E-03
    mu          0.0000      +-  0.0000
    mud1        2.7425      +-  5.23689E-03
    mud2        2.7509      +-  5.24489E-03
    ESCAPE      3.37000E-03  +-  1.83576E-04
   ====================
```

```
 Parameters (global)
 ===================
           1.0000
  CD        0.10000
  Zmin       1.00000E-06
  Zmax      -1.00000E-06
  Ethermal   0.50000
  Z1        -10.000
  Z2         10.000

Total number of events =  100000
 Energy  Total =     337  Mean = 4.621E-02 MSR = 5.784E-02  EscE

 Energy  Total =      60  Mean = 4.700E-02 MSR = 5.772E-02  EscEw

 Time    Total =   89562  Mean =  1.63    MSR =  2.07     DecT

 Range   Total =   99445  Mean = 0.265    MSR = 0.320     DecR

 Range   Total =   40761  Mean = 0.338    MSR = 0.380     DecRw

 Energy  Total =   33924  Mean = 0.413    MSR = 0.509     mud1e2

 Energy  Total =   65975  Mean = 0.409    MSR = 0.507     mud2e2

 Energy  Total =   38376  Mean = 4.171E-02 MSR = 5.295E-02  mud1e30

 Energy  Total =   60067  Mean = 3.886E-02 MSR = 4.948E-02  mud2e30

 Time    Total = 11984726  Mean = 0.622    MSR = 0.716     mud1t

 Time    Total =  7359131  Mean = 0.509    MSR = 0.630     mud2t

 Time    Total = 11292595  Mean = 0.624    MSR = 0.717     mud1tw01

 Time    Total =  7048506  Mean = 0.514    MSR = 0.633     mud2tw01

You may delete "PAUSE" in C:\Mucat\SCR\MUC_4.bat if running is OK.
Press any key . . .

--------------------------------------------------------------------------
```

This pause is arranged in MUC_4.bat file for the user to check if the running is normal. Just press any key and the final operation will be performed:

```
--------------------------------------------------------------------------


Directory already exists
      1 file(s) copied
EscE.MCK
EscEw.MCK
DecT.MCK
DecR.MCK
DecRw.MCK
mud1e2.MCK
mud2e2.MCK
mud1e30.MCK
mud2e30.MCK
mud1t.MCK
mud2t.MCK
mud1tw01.MCK
mud2tw01.MCK
      13 file(s) copied
--------------------------------------------------------------------------
```

Then close the window with the MS-DOS session.

The results of the calculation will be written in a subdirectory named after the kinetics definition file. In the example, this will be C:\Mucat\Run\test\Hot. The archive contains 13 result files *.DAT and one Hot.SUM calculated with 10^5 events. You may like to save them before running your own version and check that you can reproduce them.

Here is an extract from the summary file Hot.SUM:

```
--------------------------------------------------------------------------
```

```
   Monte Carlo Kinetics v.10  MIA March-2002
 *** FCN library from C:\Mucat\FCN\fcn_4
 Hot.kin

STATES ----------
   0  DECAY       0   0     0   3
   1  mu          2   1     0   0
   2  mud1        2   3     1   0
   3  mud2        2   5     2   0
   4  ESCAPE      0   0     0   1
PARAMETERS ----------
   0          1.000E+00
   1  CD       1.000E-01
   2  Zmin     1.000E-06
   3  Zmax    -1.000E-06
   4  Ethermal  5.000E-01
   5  Z1      -1.000E+01
   6  Z2       1.000E+01
FUNCTIONS ----------
   0           1   0
   1  Mud_e1      1  406
   2  dd11        1  201
   3  dd12        2  201
   4  dd21        3  201
   5  dd22        4  201
TRANSITIONS ----------
   1     1   2     1       2    3.333E+07
   2     1   3     1       0    6.667E+07
   3     2   2     2       4    1.000E+00
   4     2   3     3       0    1.000E+00
   5     3   2     4       6    1.000E+00
   6     3   3     5       0    1.000E+00
VOLUMES ----------
   1: Target       1    5 -1.000E+01   6  1.000E+01      2   3
        Local Parameters:
          None
   2: VACUUM 1     0     0 -1.000E+19   5 -1.000E+01      0   1
        Local Parameters:
          None
   3: VACUUM 2     0     6  1.000E+01   0  1.000E+19      1   0
        Local Parameters:
          None
POPULATIONS ----------
   1     2       3    mud1e2          2     2.000E-03     0
          0.000E+00  2.500E-01  5.000E-03    0.000E+00  0.000E+00
   2     3       4    mud2e2          2     2.000E-03     0
          0.000E+00  2.500E-01  5.000E-03    0.000E+00  0.000E+00
   3     2       5    mud1e30         2     3.000E-02     0
          0.000E+00  5.000E+00  5.000E-02    0.000E+00  0.000E+00
   4     3       6    mud2e30         2     3.000E-02     0
          0.000E+00  1.000E+00  1.000E-02    0.000E+00  0.000E+00
   5     2       7    mud1t           1     0.000E+00     0
          0.000E+00  1.000E+00  1.000E-02    0.000E+00  0.000E+00
   6     3       8    mud2t           1     0.000E+00     0
          0.000E+00  0.000E+00  0.000E+00    0.000E+00  0.000E+00
   7     2       0    mud1tw01        1     0.000E+00     1
          0.000E+00  0.000E+00  0.000E+00    0.000E+00  1.000E-01
   8     3       0    mud2tw01        1     0.000E+00     1
          0.000E+00  0.000E+00  0.000E+00    0.000E+00  1.000E-01
YIELDS ----------
   1     0   4     0       2    EscE            2     0
          0.000E+00  2.500E-01  5.000E-03    0.000E+00  0.000E+00
                                0.000E+00  0.000E+00
   2     0   4     0       0    EscEw           2     2
          0.000E+00  2.500E-01  5.000E-03    0.000E+00  0.000E+00
                                1.000E+01  2.000E+01
   3     0   0     0       4    DecT            1     0
          0.000E+00  5.000E+00  5.000E-02    0.000E+00  0.000E+00
                                0.000E+00  0.000E+00
   4     0   0     0       5    DecR            4     0
          0.000E+00  1.000E+00  1.000E-02    0.000E+00  0.000E+00
                                0.000E+00  0.000E+00
   5     0   0     0       0    DecRw           4     3
          0.000E+00  1.000E+00  1.000E-02    0.000E+00  4.000E-02
                                1.000E+00  1.000E+01
Number of States    :  4
Number of Links     :  6
Number of Parameters :  6
Number of Functions  :  5
```

```
 Number of Media     :  1
 Number of Volumes   :  3
 Initial state  :  1
 Ncollision_max :   65535
 T_max        :  2.000E+01
 Decay rate    :  4.550E-01

 Scattering angles and coordinates are calculated
Hote media model is implemented for  temperature 300.0K
below lab. kinetic energy  0.50eV
Cold media model is implemented above
                                22-APR-03  20:12:57
   Hot.kin
    Number of events =   100000
   ============
   Total yields
   ============
    DECAY       0.99660     +-  3.15690E-03
    mu          0.0000      +-   0.0000
    mud1        2.7425      +-  5.23689E-03
    mud2        2.7509      +-  5.24489E-03
    ESCAPE      3.37000E-03  +-  1.83576E-04
   ===================
   Parameters (global)
   ===================
              1.0000
    CD         0.10000
    Zmin        1.00000E-06
    Zmax       -1.00000E-06
    Ethermal    0.50000
    Z1         -10.000
    Z2          10.000
   =============
   Transitions
   =============
    EscE          Energy      3.370E-03     4.621E-02   5.784E-02
    EscEw          Energy      6.000E-04     4.700E-02   5.772E-02
    DecT          Time        0.896         1.63        2.07
    DecR          Range       0.994         0.265       0.320
    DecRw          Range       0.408         0.338       0.380
   =============
   =============
   Populations
   =============
    mud1e2         Energy      0.339         0.413       0.509
    mud2e2         Energy      0.660         0.409       0.507
    mud1e30         Energy      0.384         4.171E-02   5.295E-02
    mud2e30         Energy      0.601         3.886E-02   4.948E-02
    mud1t          Time        120.          0.622       0.716
    mud2t          Time        73.6          0.509       0.630
    mud1tw01        Time         113.          0.624       0.717
    mud2tw01        Time         70.5          0.514       0.633
   =============
--------------------------------------------------------------------------
```

Almost all results have been illustrated in the section 3.3 “The structure of output information”.

The target, filled with pure D_2 at 0.05 LHD, has only one volume 'Target', which has a the form of a cylinder with 1 mm radius and 20 mm length. 10^5 muons stop in the center of the volume, forming dμ atoms in the natural proportion (1:2) of populations of the two spin states $d\mu_{1/2}$ and $d\mu_{3/2}$. The initial energy distribution of dμ atoms has a sharp peak at the energy of 1 eV; that is defined in Mud_e1.fcn file. The reactions of elastic scattering, defined by dd11.fcn and dd22.fcn, and the spin-flip, defined by dd12.fcn and dd21.fcn, are possible. The corresponding *.fcn files contain the rates for the reactions on D, but the masses of media particles are the doubled masses of D. The density 0.1 LHD for D corresponds to the 0.05 LHD of D_2.

So, the dμ atoms diffuse in D_2 until they escape the volume or the muons decay. The file DecT.dat gives the time distribution (counts /50ns) of all decays that had occurred in the time interval [0., 5.] mks. The summary file Hot.SUM shows that 89.6% of all muons had decayed in that time interval, the mean decay-time being 1.63 mks and the mean squared time 2.07 mks. The file EscE.dat gives the energy distribution (counts /0.005eV) of dμ atoms escaping from the volume. The file EscEw.dat gives the same distribution in the time interval [10., 20.] mks;

0.337% of all mesic atoms escape from the target with their energy in the interval [0., 0.25] eV, and only 0.06% have that energy and escape during this time interval, etc. The file mud2e2.dat gives the energy distribution of $d\mu_{3/2}$ atoms at 2 ns in the energy interval [0., 1.2] eV. The summary file says that 66% of all muons are in this state at 2 ns and have the energy in this interval. And their mean energy is 0.409 eV, etc.

Compare the end of the file Hot.SUM with the extraction from the file Hot.kin:

```
'*POPULATION'
   'mud1'   'Energy'  0.002  0.0 1.2 0.01   0. 0.   'mud1e2'
   'mud2'   'Energy'  0.002  0.0 1.2 0.01   0. 0.   'mud2e2'
   'mud1'   'Energy'  0.03  0.0 0.2 0.001   0. 0.   'mud1e30'
   'mud2'   'Energy'  0.03  0.0 0.2 0.001   0. 0.   'mud2e30'
   'mud1'   'Time'     0.0   0.0 1.275 0.005   0. 0.  'mud1t'
   'mud2'   'Time'     0.0   0.0 1.275 0.005   0. 0.  'mud2t'
   'mud1'   'Time'     0.0   0.0 1.275 0.005  0. 0.1  'mud1tw01'
   'mud2'   'Time'     0.0   0.0 1.275 0.005  0. 0.1  'mud2tw01'
   'END'    'END'    0.    0. 0. 0.00  0. 0.   'END'
'*YIELD'   Calculated distributions
  ' '  '->' 'ESCAPE'  ' '  'Energy'   0. 0.25 0.005  0.0 0.0   0. 0.  'EscE'
  ' '  '->' 'ESCAPE'  ' '  'Energy'   0. 0.25 0.005  10. 20.  0. 0.  'EscEw'
  ' '  '->' 'DECAY'  ' '  'Time'    0. 5.0  0.05   0.0 0.0   0. 0. 'DecT'
  ' '  '->' 'DECAY'  ' '  'Range'    0. 1.0  0.01   0.0 0.0   0. 0. 'DecR'
  ' '  '->' 'DECAY'  ' '  'Range'    0. 1.0  0.01   1. 10.  0. 0.04 'DecRw'
 'END'  '->'  'END'  'END'  'END' 0. 0. 0.  0. 0.  0. 0. 'END'
```

The thermal energy in Hot.kin is 0.5 eV, that is 1/2 of the initial dμ energy. This is to implement both the both the "Hot media" and the "Cold media" models. The run below tests the old version (v.9) of the code with the "Cold media" model only. The file Cold.kin is a copy of the Hot.kin with different name only. The parameter 'Ethermal' is ignored there. The way of running is the same:

```
>cd C:\Mucat\Run\test
>runV9
```

Then you should type 100000:

```
running Mucat9.exe
   >>> Number of events = 100000
```

and wait for the calculation:

```
   *** Kinetics definition completed
   *** Wait please. Calculating kinetics ...
   |--------------------|
   |.......
```

And the resulting files there are in the subdirectory C:\Mucat\Run\test\Cold.

C. Several examples of MUCAT usage.

C.1 Kinetics of dμ in D2 gas.

A muon stops in the unlimited area with D_2 gas at temperature 300 K and density 0.05 LHD, forming instantly dμ atoms with initial kinetic energy 1 eV. The two spin states $d\mu_{1/2}$ and $d\mu_{3/2}$ are formed in the natural proportion 1:2. These mesic atoms scatter on the molecules of media, elastic scattering and the spin-flip are possible. The effective scheme of kinetics is drawn below. The effective rates for the ddμ formation are used, with back-decay processes taken into account. The muon sticking process

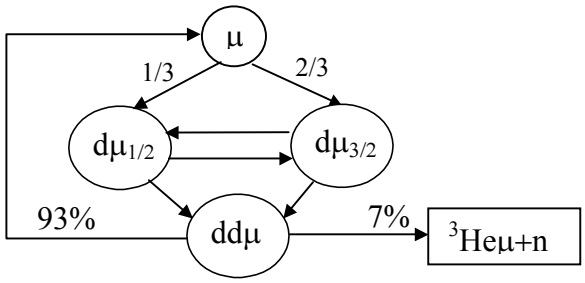
$dd\mu \rightarrow {}^3He\mu + n$

has 7% probability with respect to all other syntheses:

$dd\mu \rightarrow {}^3He + n + \mu$

$dd\mu \rightarrow t + p + \mu$

The synthesis is considered to be instant.



Effective kinetics scheme for dμ in D_2

It is required to obtain:

1) Time spectra of ddμ formation in the intervals [0,10] mks and [0,100] ns.
2) Energy distribution of dm atoms at 10 ns and 100 ns.
3) Average energy of dμ atoms versus time in the interval [1,100] ns.

To solve this task the following steps should be done. They were done before and all the necessary files were included in 'Mucat' archive, meanwhile one can repeat all the steps again with detailed explanations.

1. Create the subdirectory dmu_D2 in the directory C:\Mucat\Run. Then create the Kinetic definition file main.kin there: C:\Mucat\Run\ main.kin, with the following contents.

```
'*TITLE' main.kin Kinetics of mud in D2 Gas at T=300
 'main.kin'
'*SHOW'
     3
'*PARAMETER'
     'CD2'
     'Zmin'
     'Zmax'
     'Ethermal'
     'END'
'*LET'
     'CD2'    0.05
     'Zmin'   1.e-6       Compact source
     'Zmax'  -1.e-6
     'Ethermal'  1000.       eV, below new algoritm is
     'END' 0.
'*STATE'
     'mu'
      'mud1'           initial energy  E = 1.0 eV
      'mud2'
        'mudd'
         'stick'
     'END'
'*INITIAL'
     'mu'
'*LINK'
  'mu' '->' 'mud1' 0.3333E8    'Mud_e1'  very fast
  'mu' '->' 'mud2' 0.6667E8    'Mud_e1'
     'mud1'   '->'   'mud1'   1.   'GRDDD11'
     'mud1'   '->'   'mud2'   1.   'GRDDD12'
     'mud2'   '->'   'mud1'   1.   'GRDDD21'
     'mud2'   '->'   'mud2'   1.   'GRDDD22'
       'mud1'   '->'   'mudd'   1.   'ddmd1'
       'mud2'   '->'   'mudd'   1.   'ddmd3'
                'mudd'   '->'   'mu'   0.93E15   ' '
                'mudd'   '->'   'stick'   0.07E15   ' '
```

```
     'END' '->'   'END'     0.     'END'
'*DECAY'
      0.455    Decay rate in units of 1/mks
 '*TIME'       Maximum time
      20.
'*POPULATION'
  'mud1'   'Energy'   0.01  0.0 1.2 0.005   0. 0.   'mud1e10'
  'mud2'   'Energy'   0.01  0.0 1.2 0.005   0. 0.   'mud2e10'
  'mud1'   'Energy'   0.1  0.0 1.2 0.005   0. 0.   'mud1e100'
  'mud2'   'Energy'   0.1  0.0 1.2 0.005   0. 0.   'mud2e100'
  'END'    'END'    0.    0. 0. 0.00  0. 0.   'END'
'*YIELD'   Calculated distributions
 ' ' '->' 'mudd' ' '   'Time '   0. 10.0 0.1  0.0 0.0  0. 0.  'mddyt10'
 ' ' '->' 'mudd' ' '   'Time '   0. 0.1 0.001  0.0 0.0  0. 0.  'mddyt0_1'
 'END'  '->'  'END'  'END'  'END'    0.  0.  0.    0.  0.   0. 0.  'END'
'*END'   End of kinetics definition
```

The list **'*TITLE'** is obvious and comprises the file title **'main.kin'**. The next list is also a formal one: **'*SHOW'**. Number **3** defines the information volume that is output to the screen during the code running. The next list **'*PARAMETER'** includes the parameter **'Ethermal'**, which is defined in the next list **'*LET'**. The value of this parameter is taken large enough to be higher than the right edge value of the 101-point energy grid: C:\Mucat\Grids\ENERG101.txt, which is 105.75 eV. This is not to be implemented at all for the "Cold media" model. The other parameters will be introduced a bit later.

The list of available states **'*STATE'** includes the names according to the effective kinetic scheme, mentioned above.

'mu'	μ
'mud1'	$d\mu_{1/2}$
'mud2'	$d\mu_{3/2}$
'mudd'	$dd\mu$
'stick'	$^3He\mu+n$

To set the initial dμ energy distribution, the state **'mu'** is indicated in the list **'*INITIAL'** and then the first two lines of the list **'*LINK' are introduced**, corresponding to the first generation of the muon evolution. File **'Mud_e1.fcn'** of the class **'1->2'** should be created for this purpose.

2. Create subdirectory fcn_2 in C:\Mucat\fcn\, then copy the file C:\Mucat\fcn\fcn_1\Mud_e1_2.fcn into C:\Mucat\fcn\fcn_2\Mud_e1.fcn and edit the latter. All you need to change is two columns in the end of the file that correspond to the energy distribution, and the density parameter. You can also replace the label **'Z'** with the blank **' ',** in order not to redefine the muon position in every muon atomic capture. The file Mud_e1.fcn becomes as it is shown below:

```
'1->2 W  '          Atomic capture mu->mud       mud_e1.FCN  March 2003
 'CD2     '                  ***  Limited z-range  ***
 1.e7                        ***  Isotropic        ***     Very Fast ***
 1981.287e6    ***  Delta  1.00 eV  ***
 'Zmin    '
 'Zmax    '
 -1.
  1.
  0.
  6.28318
     0.    0.
     0.999 0.
     1.000 1.
     1.001 0.
     2.0   0.
     10.   0.
```

3. After creation of Mud_e1.fcn it is clear that the density parameter **'CD2'** and the muon stop boundaries **'Zmin'** and **'Zmax'** must be declared in main.kin. They must be mentioned in the list **'*PARAMETER'** and their values are defined in the list **'*LET'**. So, according to the task definition, **'CD2'** must be equal to **0.05** and it does not matter what value **'Zmin'** and **'Zmax'** have. The rate **1.e7** mks^{-1} from Mud_e1.fcn will be multiplied **0.3333E8** or **0.6667E8** from main.kin providing very fast transitions in the natural ratio of probabilities 0.3333E8 : 0.6667E8 = 1 : 2.
Turning back to the list **'*LINK'** in main.kin, compose the next four lines of the second generation. They describe the elastic scattering and the spin-flip reaction of dμ atoms on media molecules D_2. The statistical weight of the final states is **1.** for these transitions. Corresponding files **'GRDDD*.fcn'** of the class **'2->2'** have to be created. They must include the multiplicative density parameter **'CD2'**. The next two lines of the list **'*LINK'** also belong to the second generation of the kinetic scheme. They stand for the reactions of ddμ formation. The statistical weights are also **1.** and corresponding files **'ddmd1.fcn'** and **'ddmd3.fcn'** must include parameter **'CD2'** and be of the class **'2->1'**. The third generation is all reactions of the synthesis. The statistical weight of **'stick'** is **0.07** and the synthesis rate is **1E15** mks^{-1}.
The real decay rate **0.455** mks^{-1} is indicated in the simple list **'*DECAY'**. The maximum cycle time 20 mks stands in **'*TIME'**.

The energy distributions of $d\mu_{1/2}$ and $d\mu_{3/2}$ atoms at 10 ns and 100 ns is required in the list **'*POPULATION'**. The time spectra of ddμ formation in the intervals [0,10] mks and [0,100] ns is required in the list **'*YIELD'**. The names of files with output information (here they are **'mud1e10.dat'**, **'mud2e10.dat'**, **'mud1e100.dat'**, **'mud2e100.dat'**, **'mddyt10.dat'**, **'mddyt0_1.dat'**) should contain abbreviation of a state, a distribution type, point (time, energy, etc.) and should be not longer than 8 characters to avoid possible errors. For example,**'mud1e10.dat'**:

mud1 — the name of the state,
e — the **e**nergy distribution,
10 — the time point 10 mks;

'mddyt0_1.dat':

mdd — the name of the state,
y — taken from **y**ield,
t — the **t**ime distribution,
0_1 — the time interval [0, **0.1**] ns.

Remember that Windows makes no difference between upper- and lower-case letters.

4. Create ddmd*.fcn files. There is the file qddmd300.dat in the archive C:\Mucat\Data\DDmd.ZIP, which contains the rate of dμ dformation for dμ in D_2 gas at 300 K versus dμ energy in LAB. There are 5 columns in the file qddmd*.dat: 1 — energy of dμ atoms in eV; 2 and 3 — the absolute and effective rates, with back-decay included, for the reaction $d\mu_{1/2} + D_2 \rightarrow dd\mu$; 3 and 4 — the absolute and effective rates for $d\mu_{3/2} + D_2 \rightarrow dd\mu$. So, the columns 1, 3, 5 are needed. Corresponding rates are drawn in the figure below.

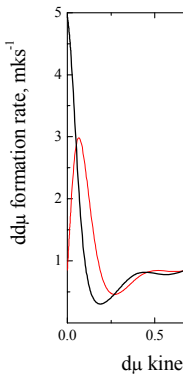


Fig. ddμ formation rate for d

The corresponding files ddmd*.fcn must contain the header '2->1', the multiplicative parameter 'CD2', the edges of the energy range Emin and Emax and two columns with the energies and rates. These columns should not be longer than 250 rows. Below there is an extraction from the file ddmd1.fcn:

```
'2->1  0 '   ddmu formation mud(1/2)+D2(T=300 K), molecule stops   03/31/03
 'CD2   '  0.   2.00   File is created by 'FCN21CREATION' from 'qddmd300.dat'
 0.100000E-03  0.850858E+00
 0.400000E-03  0.864411E+00
 0.700000E-03  0.878075E+00
          …              …
0.199000E+01  0.153422E+01
```

There is a special tool in C:\Mucat\Tool\ FCN21Creation that creates ddmd*.fcn from the file qddmd*.dat. To use it, you have to copy the file qddmd300.dat to C:\Mucat\Tool\ FCN21Creation, then double click FCN21Creation.dsw (if Visual Fortran 6.0 is installed on the computer. If not, then compile the program FCN21CREATION.for and run the executable file.) Then press "Build// Execute FCN21Creation.exe", answer "Yes" to the question "Do you want to build FCN21Creation.exe", and FCN21Creation.exe will run. Just follow the instructions. When you see the invitation

Type '1' for 30K and '2' for 300K

Then type

2

and press <Enter>.

Then you see:

Type '1' for md(1/2) and '2' for md(3/2)

The code has to be run twice with both variants. So type

1

(and type **2** for the second running)

and press <Enter>.

Then the pause will appear:

749 rows read

Number of rows > 250.   Press <ENTER>

This message appears because the file qddmd300.dat contains more than 250 rows. So, every third row will be written into ddmd1_300.fcn or ddmd3_300.fcn. After these two executions, the files ddmd1_300.fcn and ddmd3_300.fcn should be renamed into ddmd1.fcn and ddmd3.fcn respectively and copied to C:\Mucat\fcn\fcn_2.

5. Create GRDDD*.fcn files.

There were no *.fcn files for $d\mu+D_2 \rightarrow d\mu+D_2$. There are data with differential rates and cross sections in LAB system at temperature 300 K in the archive C:\Mucat\ Data\ DATA300K.zip. This data has been obtained with the averaging weight

$$\boldsymbol{f(E_b, \cos\xi)} = \tfrac{1}{2} f_M(E_b),$$

instead of

$$\boldsymbol{f(E_b, \cos\xi)} = \tfrac{1}{2} f_M(E_b) \frac{\lambda(E_{coll})}{\lambda(E_a)},$$

which is derived in section 5.1 of this manual. Therefore the differential rates seem to give more realistic results than those with the cross sections.

It is easy to create GRDDD*.trm files from DATA300K.zip\ GRDDD*.300.ZIP\ GRDDD*.300. Just insert the header:

```
300.0 K   double diff. rates in lab. system
Energy channels from ENERG101.txt
InEn FinEn Theta ddSigma
```

and put the result into C:\Mucat\fcn\fcn_2\ GRDDD*.trm. Then the code needs the header of GRDDD*.fcn:

```
'2->2   '
```

'CD2 ' 5
1981.287e6 3752.256e6 1981.287e6 3752.256e6 0.0 0.00 100.

Place all the GRDDD*.fcn with this contents also into C:\Mucat\fcn\fcn_2\. Usually, the code creates *.trm file from *.fcn, but the files GRDDD*.fcn do not contain necessary information. Fortunately, in this particular case it is possible to create GRDDD*.tra with the rates from GRDDD*.trm with differential rates. For this purpose, the code MUCAT with a small change can be used. All the necessary files GRDDD*.tra have been created and placed properly. If you want to reproduce them, you can uncomment 10 lines starting from "cw" in the file C:\Mucat\fort\ src10\ kfcn.for, by deleting those "cw". Then compile the code. Remove the previous versions of GRDDD*.tra and run the code. It will run as usually and will not stop after creation of *.tra, but do not forget to put back in place these comments "cw" in kfcn.for and recompile the code again for further usage.

6. Create C:\Mucat\ Run\ dmu_D2\runmain.bat to run the script C:\Mucat\scr\ MUC_2.bat with the Kinetic definition file C:\Mucat\ Run\ dmu_D2\main.kin. It has to contain the following:
..\..\Scr\MUC_2.bat main
Then it is better to change the properties of runmain.bat. Click with the right button of the mouse on the file and choose "Properties…", then click the bookmark "Memory", and set "Environment variables" to 1280.

7. Create C:\Mucat\ scr\ MUC_2.bat, which sets
BASE = C:\Mucat
FCNLIB=%BASE%\FCN\fcn_2
and runs the code
%BASE%\Project\MUCAT10\Debug\Mucat10.exe
It is easy to create it from C:\Mucat\scr\ MUC_1.bat, editing principally these three lines.

8. Run the code.
The execution time on a computer with 1.4 GHz AMD processor is about 11 min.
Put the cursor onto C:\Mucat\Run\ dmu_D2\runmain.bat and press <Enter>. Then press any key when it is required. Type 1000000 when the prompt appears:
>>> Number of events =
and press <Enter>.
The directory C:\Mucat\Run\dmu_D2\main contains results for the number of events equal to 10^6. When the run finishes, the files *.dat and main.sum are overwritten.

9. The results can be illustrated in the Origin project. There is one ready in C:\Mucat\Run\dmu_D2\main\AvDmuEn.OPJ.

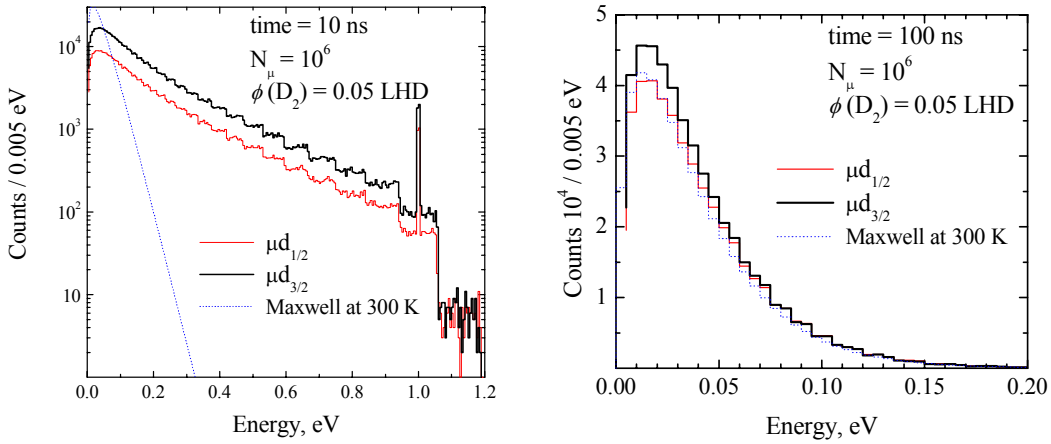


Fig. Energy distribution of dμ atoms at 10 ns and 100 ns.

The data plotted on this figure are taken from the files mud1e10.DAT, mud2e10.DAT (for 10 ns) and mud1e100.DAT, mud2e100.DAT (for 100 ns).

The Maxwellian distribution here has been obtained using the tool C:\Mucat\Tools\Maxwell. Unpack the archive Maxwell.zip into this subdirectory and edit the file Maxwell.for as necessary. There are 3 values to be changed: N — the total number of particles, emax — the maximum energy of the distribution in eV (minimum energy is zero), estep — the step of the distribution in eV (on the figure above estep = 0.005), and File='maxwN.dat' — the name of the output file. N is determined, for instance, in the Origin project, by integration of the energy distribution and multiplying by the energy step. For the energy distribution at 10 ns, N was equal to 448410, and for the distribution at 100 ns N = 346745.

Compile the programs Maxwell.for and Gauss.for and run executable Maxwell.exe. Then you will see:

OK!

Press any key to continue

Now you can move the created file C:\Mucat\Tools\Maxwell\maxw*.dat to C:\Mucat\Run\dmu_D2\main. The output file maxw*.dat contains three columns: 1 — the right edge of the energy bin, 2 — the Maxwellian probability density, and 3 — the Maxwellian probability. On the figures above, the third column has been plotted versus the first.

The data from mddyt0_1.DAT and mddyt10.DAT are plotted on the following figure.

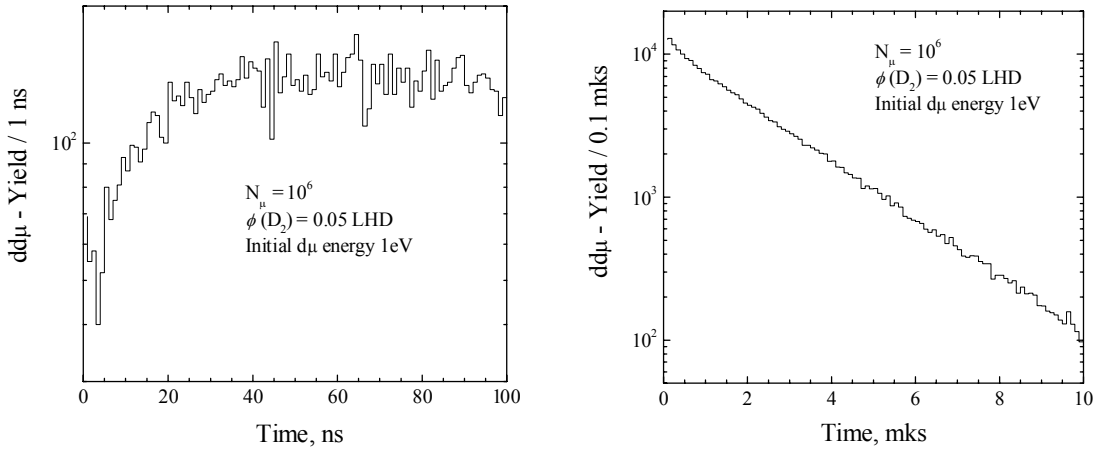


Fig. Time spectra of ddμ formation.

10. To calculate the average energy of dμ atoms versus time in the interval [1,100] ns, look at the end of main.SUM:

==========

```
Populations
============
 mud1e10       Energy     0.348       0.187      0.268
 mud2e10       Energy     0.647       0.186      0.267
 mud1e100      Energy     0.458       4.139E-02  5.528E-02
 mud2e100      Energy     0.496       4.009E-02  5.558E-02
============
```

There is the average energy of dμ atoms in the fourth column for the moments of time 10 ns and 100 ns. To obtain other points, one has to insert several additional lines into the list **'*POPULATION'** of main.kin. As the maximum number of lines in this list is equal to 8, the new kinetic definition file is to be created. Copy the file main.kin into dm1ener.kin and edit the latter. Completely remove the list **'*YIELD'** and change the list **'*POPULATION'** as follows:

```
'*POPULATION'
  'mud1'   'Energy'   0.001  0.0 1.2 0.005   0. 0.   'mud1e1'
  'mud1'   'Energy'   0.003  0.0 1.2 0.005   0. 0.   'mud1e3'
  'mud1'   'Energy'   0.005  0.0 1.2 0.005   0. 0.   'mud1e5'
  'mud1'   'Energy'   0.02  0.0 1.2 0.005   0. 0.   'mud1e20'
  'mud1'   'Energy'   0.03  0.0 1.2 0.005   0. 0.   'mud1e30'
  'mud1'   'Energy'   0.04  0.0 1.2 0.005   0. 0.   'mud1e40'
  'mud1'   'Energy'   0.05  0.0 1.2 0.005   0. 0.   'mud1e50'
  'mud1'   'Energy'   0.07  0.0 1.2 0.005   0. 0.   'mud1e70'
  'END'    'END'    0.    0. 0. 0.00  0. 0.   'END'
```

Make rundm1en.bat from runmain.bat, replace **main** with **dm1ener**, change the property of rundm1en.bat as previously and execute it. The subdirectory dm1ener will be created (if you have not deleted the original version of this subdirectory, then its files will be overwritten). For the particular task the end of dm1ener.SUM is needed:

```
============
Populations
============
 mud1e1        Energy     0.335       0.801      0.858
 mud1e3        Energy     0.338       0.534      0.640
 mud1e5        Energy     0.341       0.375      0.487
 mud1e20       Energy     0.362       8.533E-02  0.121
 mud1e30       Energy     0.376       5.933E-02  7.998E-02
 mud1e40       Energy     0.389       4.995E-02  6.671E-02
 mud1e50       Energy     0.402       4.583E-02  6.067E-02
 mud1e70       Energy     0.426       4.279E-02  5.713E-02
============
```

These data are for $d\mu_{1/2}$ atoms. Similar operations should be done for $d\mu_{3/2}$ atoms. Make rundm2en.bat, run it and make an extraction from C:\Mucat\Run\dmu_D2\dm2ener\dm2ener.SUM.

The results are drawn in the figure below.

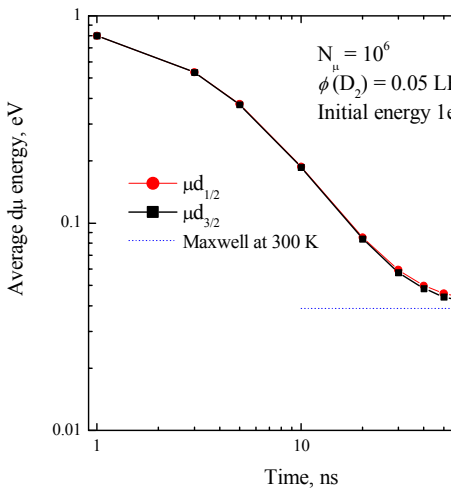


Fig. The time dependence of average dμ

C.2 The kinetics of dμ in protium gas.

A muonic atom dμ with initial energy 10 eV moves in the boundless media consisting of protium with density 0.1 LHD at 300 K, until the muon decays. Let the elastic scattering dμ+p→dμ+p be the only possible reaction. The problem is to obtain the coordinates of muon decay, i.e. the distance, which the dμ passes during the muon lifetime.

Create the file C:\Mucat\Run\Examples\mud_p_H.kin with the contents as below.

```
'*TITLE' mud_p_H.kin mud+p->mud+p  'Ethermal'  1000. 'DECAY'  '  '  'Range '
  'mud_p_H.kin'
 '*SHOW'
       3
 '*PARAMETER'
       'CP'
       'CD2'
       'Zmin'
       'Zmax'
       'Ethermal'
       'END'
'*LET'
       'CP'    0.1
       'CD2'    1.
       'Zmin'   1.e-6       Compact source
       'Zmax'  -1.e-6
       'Ethermal'  1000.       eV, below new algoritm is
       'END' 0.
 '*STATE'
       'mu'
         'mud'           initial energy  E = 10.0 eV
       'END'
'*INITIAL'
       'mu'
 '*LINK'
    'mu' '->' 'mud' 1.E8    'Mud_e10'
       'mud'   '->'   'mud'   1.   'Mud_p'
       'END' '->'   'END'     0.     'END'
 '*DECAY'
        0.455    Decay rate in units of 1/mks
  '*TIME'      Maximum time
        20.
 '*YIELD'   Calculated distributions
   '  '  '->' 'DECAY'  '  '  'Range '   0.  40. 0.5  0.0 0.0  0. 0.  'DR_Hot'
  'END'  '->'  'END'  'END'  'END' 0. 0. 0.  0. 0.  0. 0. 'END'
'*END'   End of kinetics definition
```

The parameter **'CD2'** is used only for the atomic capture of muon, $\mu+D_2\rightarrow d\mu$, and this reaction sets the initial energy of the dμ atom. The corresponding line of the list **'*LINK'**

```
    'mu' '->' 'mud' 1.E8    'Mud_e10'
```

refers to the file Mud_e10.fcn. This file is a copy of C:\Mucat\fcn\fcn_2\Mud_e1.fcn, but with another energy distribution:

```
 1.    0.
 9.99  0.
10.00  1.
10.01  0
12.    0.
```

The difference between the spin states of dμ atoms is ignored, hence possible reactions on p-atoms are written as

```
       'mud'   '->'   'mud'   1.   'Mud_p'
```

The file Mud_p.fcn contains the protium density **'CP'** as a multiplicative parameter, and describes a function of the class '2->2'.

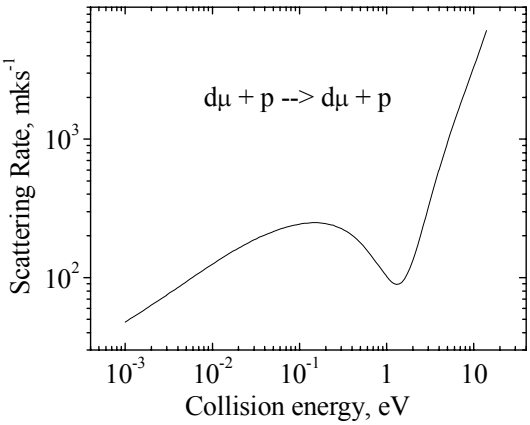


Fig. Scattering rate of dm on p

The list **'*YIELD'** requires to output the distribution of distances of muon decays into the file DR_Hot.dat.

Create the subdirectory C:\Mucat\fcn\fcn_3 and copy the file Mud_p.fcn there from C:\Mucat\fcn\fcn_1. Create Mud_e10.fcn also in fcn_3 as has been mentioned above. Then create the file C:\Mucat\scr\MUC_3.bat from MUC_1.bat, changing the FCN library:

```
SET FCNLIB=%BASE%\FCN\fcn_3
```

Then create C:\Mucat\Run\ Examples\ mud_p_H.bat:

```
..\..\Scr\MUC_3.bat mud_p_H
```

edit it if necessary to increase the environment space, and run it.

If you want to rebuild Mud_p.trm, then delete its archive version from C:\Mucat\fcn\fcn_3 before running.

Type **1000000** for the number of events and **300.** for the temperature. Then you see:

```
*** File Mud_p   .tra creation starts
 *** Opening file *C:\Mucat\FCN\fcn_3\Mud_p.tra *
 **** You should rename or delete file Mud_p   .tra containing reaction rates
Press "Enter" when ready
```

This error is due to absence of the file Mud_p.trm, when Mud_p.tra exists. Creation of *.tra is much faster than of *.trm, therefore *.tra is recreated during creation of the *.trm. Remove C:\Mucat\FCN\fcn_3\Mud_p.tra and press <Enter>. It will be recreated. Then you see:

```
*** Opening file *C:\Mucat\FCN\fcn_3\Mud_p.tra *
 Calculation CMS-->Lab starts

  Energy grid number
          1       of       101
          2       of       101
         ...      ...      ...
        101       of       101
 *** Opening file *C:\Mucat\FCN\fcn_3\Mud_p.trm *

 CMS-->Lab performed successfully

...      ...      ...        ...

Scattering angles and coordinates are calculated
Hote media model is implemented for  temperature 300.0K
   *** Kinetics definition completed
   *** Wait please. Calculating kinetics ...
   |--------------------|
   |..
```

After this run the file C:\Mucat\Run\Examples\mud_p_H\DR_Hot.DAT with the distribution of ranges is written. This distribution (hot media, T=300K) is plotted in C:\Mucat\Run \Examples\mud_p_H \Range.OPJ and it is shown on the figure below as well as the same distribution, obtained in the framework of the “Cold media” model.

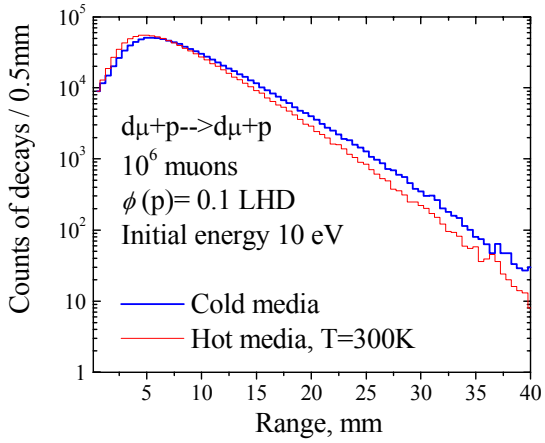


Fig. Distribution of decays on distance from a muon stop.

To obtain the latter, one has either to delete the parameter **'Ethermal'** from the file mud_p_H.kin or set it to be **0**. Then save this file as mud_p_C.kin and also edit the running file mud_p_H.bat, and save it as mud_p_C.bat:

```
..\..\Scr\MUC_3.bat mud_p_C
```

After starting of C:\Mucat\Run\Examples\mud_p_C.bat and entering the number of events equal to10^6, you will see:

```
Scattering angles and coordinates are calculated
Cold media model is implemented
   *** Kinetics definition completed
   *** Wait please. Calculating kinetics ...
   |-------------------|
   |.......
```

The file DR_Cold.DAT with the range distribution is written into the subdirectory C:\Mucat\Run\Examples\mud_p_C.

C.3 Thermalization of globules.

Globules are some particles with constant scattering rates. Construct the corresponding file a2x.fcn and put it into the subdirectory C:\Mucat\fcn\fcn_3:

```
'2->2  X '
 'CD2      ' 5
 1981.287e6  1981.287e6  1981.287e6  1981.287e6  0.0   0.00 100.
0.5000E-02  0.2000E-18 0.5 0. 0. 0. 0.
0.5600E+00  0.2000E-18 0.5 0. 0. 0. 0.
   …              …          … .   .  .  .
0.9325E+02  0.2000E-18 0.5 0. 0. 0. 0.
0.9380E+02  0.2000E-18 0.5 0. 0. 0. 0.
```

The label **'X'** in the first line says that the file contains cross sections. The multiplicative parameter **'CD2'** is arbitrary. Colliding particles of equal masses (**1981.287e6** MeV) are considered. The scattering cross section is equal to $0.2 \cdot 10^{-18}$ cm^2 and does not depend on collision energy.

Copy Mud_e1.fcn from C:\Mucat\fcn\fcn_2 to C:\Mucat\fcn\fcn_3.

Construct the Kinetic definition file C:\Mucat\Run\Examples\Globules.kin as follows:

```
'*TITLE' Globules
  'Globules'
 '*SHOW'
       3
 '*PARAMETER'
       'CD2'
       'Zmin'
       'Zmax'
       'Ethermal'
       'END'
```

```
'*LET'
      'CD2'    1
      'Zmin'   1.e-6       Compact source
      'Zmax'  -1.e-6
      'Ethermal'  4.       eV, below new algoritm is
      'END' 0.
 '*STATE'
      'mu'
       'mud'
      'END'
'*INITIAL'
      'mu'
 '*LINK'
   'mu' '->' 'mud' 1.E8    'Mud_e1'  fast capture, init. energy 1.eV
      'mud'   '->'   'mud'   1.   'a2x'
      'END' '->'   'END'     0.     'END'
 '*DECAY'
      0.000455 Real decay rate = 0.455 1/mks
  '*TIME'      Maximum time of muon cycle
     0.1
'*POPULATION'
   'mud'   'Energy'   0.1   0.0 0.2 0.002   0. 0.   'mud_en01'
   'END'    'END'    0.    0.  0.  0.    0. 0.   'END'
 '*END'   End of kinetics definition
```

The globules here are named **'mud'** and the media density, named **'CD2'**, is **1**. The parameter **'Ethermal'** is equal to **4** eV. That is higher than initial energy (1 eV), which is set in the first line of the list **'*LINK'**.

Output of the energy distribution of globules at 100 ns is requested in the list **'*POPULATION'**. To reduce calculation time, the maximum time of a muon cycle is set to **0.1** mks. The decay rate is set 10^3 times lower than the real one, to avoid considerable loss of particles by the time when thermalization has occurred.

Construct the file C:\Mucat\Run\Examples\runGlbls.bat:

..\..\Scr\MUC_3.bat Globules

Increase its environment space if necessary and run it. If you would like to reproduce the files a2x.tra and a2x.trm, remove or rename them from C:\Mucat\fcn\fcn_3 before the run. The energy dependence of the scattering rate from a2x.tra is drawn on the following plot.

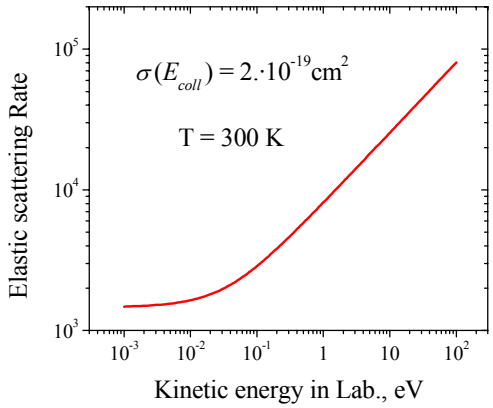


Fig. The rate of scattering with the constant cross section.

Type the number of events **1000000** and temperature **300.** when you are prompted. After CMS→LAB calculations you will see:

```
Processing without  scattering angles and coordinates calculation
Hote media model is implemented for  temperature 300.0K
below lab. kinetic energy  4.00eV
Cold media model is implemented above
   *** Kinetics definition completed
```

```
*** Wait please. Calculating kinetics ...
|--------------------|
|..
```

The energy distribution is output to C:\Mucat\Run\Examples\Globules\mud_en01.DAT. There is the Origin project GlblsMaxw.OPJ in the same subdirectory, which illustrates these results in comparison with Maxwell distribution.

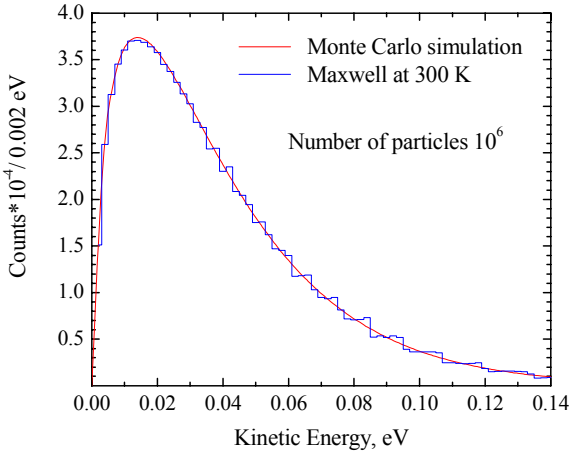


Fig. Energy distribution of thermalized globules.

The Maxwell distribution for 10^6 particles is stored in the file maxw1e6.dat. It was obtained using the tool C:\Mucat\Tools\Maxwell. To do this, edit the following lines in the file Maxwell.for:

```
Integer N/1e6/ !Number of events
Data emax/0.14/,estep/0.002/ !maximum energy and the step
OPEN(UNIT=1,File='maxw1e6.dat')
```

Compile Maxwell.for with Gauss.for and run the executable Maxwell.exe. It will create maxw1e6.dat in current directory.

C.4 Thermalization of real particles.

Let us consider thermalization of $d\mu_{1/2}$ atoms in D_2 and compare two different approaches: simulation with double differential cross sections and the same with double differential rates. The first approach is described in the section 5 and realized in the code Mucat. Integration of differential cross sections with the following weight is done during calculation CMS→LAB:

$$\boldsymbol{f(E_b, \cos\xi)} = \tfrac{1}{2} f_M(E_b) \frac{\lambda(E_{coll})}{\lambda(E_a)},$$

The following quantity is summed:

$$\tfrac{1}{2} f_M(E_b) \frac{\lambda(E_{coll})}{\lambda(E_a)} \frac{d\sigma(E_{coll})}{d\Omega} = \tfrac{1}{2} f_M(E_b) V_{rel} \frac{\sigma(E_{coll})}{\lambda(E_a)} \frac{d\sigma(E_{coll})}{d\Omega}.$$

In most of works the integration weight is the Maxwellian one:

$$\boldsymbol{f(E_b, \cos\xi)} = \tfrac{1}{2} f_M(E_b).$$

Thus integration of the following quantity is usually done:

$$\tfrac{1}{2} f_M(E_b) \frac{d\lambda(E_{coll})}{d\Omega} = \tfrac{1}{2} f_M(E_b) V_{rel} \frac{d\sigma(E_{coll})}{d\Omega}.$$

The result of this integration is called "double differential rates" and corresponds here to the second approach. There is also the third approach, where the differential cross section is summed with the Maxwellian weight:

$$\tfrac{1}{2} f_M(E_b) \frac{d\sigma(E_{coll})}{d\Omega}.$$

Usually, this is called “double differential cross sections”, but it should be appended “with Maxwell weight”.

To compare these three approaches, the energy distribution of dμ atoms should be obtained for a moment of time, when they become thermalized. This means that the energy distribution does not change any more. The dμ atoms with 1 eV initial energy in D_2 media at 0.1 LHD reach thermalization in about 100 ns. To be sure, take the moment 5 mks.

Create the directory C:\Mucat\Run\Thermal and the Kinetic definition file ddmu.kin in it.

```
'*TITLE' *** Thermalization of mud in D2 media  ddmu.kin   02/2002
 'ddmu'
'*SHOW'
      3
'*PARAMETER'
      'CD'
      'Zmin'
      'Zmax'
      'Ethermal'
      'END'
'*LET'
      'CD'    0.1
      'Zmin'  1.e-6       Compact source
      'Zmax'  -1.e-6
      'Ethermal'  1000.       eV, below new algoritm is
      'END' 0.
'*STATE'
      'mu'
       'mud1'           initial energy  E = 1.0 eV
      'END'
'*INITIAL'
      'mu'
'*LINK'
   'mu' '->' 'mud1' 1.E8    'Mud_e1'
      'mud1'   '->'   'mud1'   1.   'dd11'
      'END' '->'   'END'     0.     'END'
'*DECAY'
       0.000455    Decay rate in units of 1/mks
 '*TIME'      Maximum time
  5.01  5.  .11  20.
'*POPULATION'
   'mud1'   'Energy'    5.   0.0 0.2 0.001   0. 0.   'mud_50'
   'END'     'END'    0.     0.  0.  0.     0. 0.   'END'
'*END'   End of kinetics definition
```

Here the first line of the list **'*LINK'** stands for setting of the initial kinetic energy of dμ atoms. The corresponding file Mud_e1.fcn can be copied to fcn_4 from the subdirectory fcn_2. The second line of the list **'*LINK'** is for elastic scattering; it refers to the file dd11.fcn. Copy it from C:\Mucat\fcn\fcn_1\Mud_d11.fcn into C:\Mucat\fcn\fcn_4\dd11.fcn and change there the mass of D (**1875.628e6 eV**) to the double mass **3752.256e6** eV. Also the value of E_{cut} in the third line of dd11.fcn is to be changed from **0.04** to **0.005** eV.

The media density (**'CD'**) is equal to **0.1** LHD; this corresponds to density of D_2 0.05 LHD; the muon decay rate (**'*DECAY'**) is taken 10^3 times less than the real one, not to loose the particles. The maximum of the muon life time (**'*TIME'**) exceeds slightly the moment of time, when the population is calculated.

The list **'*POPULATION'** requests to output the energy distribution of $d\mu_{1/2}$ (**'mud1'**) into the file **mud_50.fcn**.

This Kinetic definition file ddmu.kin is for the first approach with double differential cross sections. Copy this file into ddmuAn.kin and ddmuAnx.kin in the same directory and

make the following changes: append the parameter **'CD2'**, set its value to **0.05** and edit the second line of the list **'*LINK'**:

'mud1' '->' 'mud1' 1. 'GRDDD11'

for the second approach and

'mud1' '->' 'mud1' 1. 'GXDDD11'

for the third approach.

The file C:\Mucat\fcn\fcn_4\GRDD11.fcn contains only the header:

```
 '2->2    '
 'CD2     ' 5
 1981.287e6  3752.256e6  1981.287e6  3752.256e6  0.0   0.00 100.
```

How to create GRDD11.trm and GRDD11.tra with differential and total scattering rates is described in the appendix C.1. You can copy them from C:\Mucat\fcn\fcn_2.

The file C:\Mucat\fcn\fcn_4\GXDD11.fcn also consists of only the header, but the identifier includes the label **'X'**, which says that GXDD11.trm contains cross sections, but not rates:

```
'2->2  X '
```

The file C:\Mucat\fcn\fcn_4\GXDD11.trm is created from C:\Mucat\Data\DATA300K.zip\GXDD11.300. These data are the differential cross sections in LAB, obtained by some other code with Maxwellian weight. The file GXDD11.tra is the exact copy of GRDD11.tra.

Create the three running files ddmu.bat, ddmuAn.bat, ddmuAnx.bat. They include

..\..\Scr\MUC_4 ddmu

or

..\..\Scr\MUC_4 ddmuAn

or

..\..\Scr\MUC_4 ddmuAnx

respectively. Increase their environment space if necessary, and run them consequently. After that the subdirectories ddmu, ddmuAn, ddmuAnx are created in the directory C:\Mucat\Run\Thermal. Each of them contains the file mud_50.DAT with the energy distri-

bution. There is the Origin project C:\Mucat\Run\Thermal\ddmu\Thermal.opj, which illus-

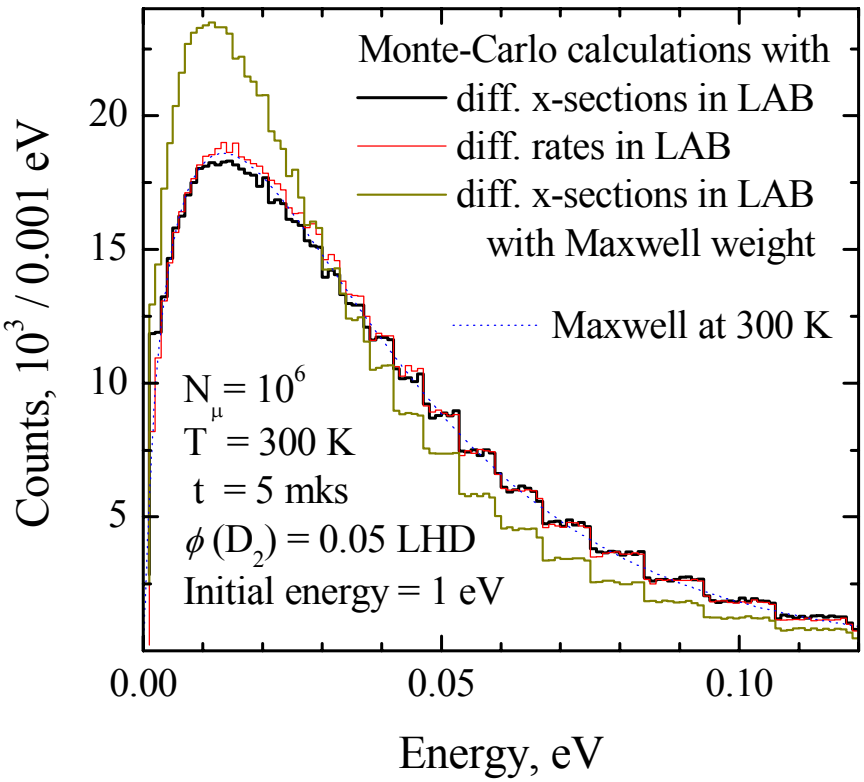


Fig. Energy distribution of $d\mu_{1/2}$ atoms after thermalization.

trates the results.

This demonstrates clearly that the third approach produces a wrong energy distribution. The first two approaches are compatible. The double differential rates give more precise mean energy **3.876E-02** eV than the double differential rates in the first approach: **3.936E-02** eV; meanwhile this value for the temperature 300 K has to be $3.88 \cdot 10^{-2}$ eV.

In the first approach better results can be obtained using more detailed energy and angle grids in CMS→LAB calculation (see section 5).

D. The model for simulation of kinetic processes.

The program simulates the trajectories of individual muons. The moment of decay is considered to be a random value, distributed in the interval $t \in (0,+\infty)$ with density

$$p(t) = \lambda_\mu e^{-\lambda_\mu t},$$

where λ_μ is the muon decay rate. The following formula is used to generate T_{dec}

$$T_{dec} = -\frac{1}{\lambda_\mu} \ln \gamma,$$

where γ is a random number uniformly distributed in the interval (0,1). Every new T_{dec} is obtained with a new γ.

The transition channel n is calculated according to the formula

$$\sum_{i=1}^{n} \lambda_i = \gamma \sum_{i=1}^{N_{tr}} \lambda_i,$$

where N_{tr} is the total number of possible transitions from the given state, λ_i is the partial rate of transition into i-th channel. The equation above should be treated as two inequalities:

$$\sum_{i=1}^{n}\lambda_i < \gamma\sum_{i=1}^{N_{tr}}\lambda_i < \sum_{i=1}^{n+1}\lambda_i .$$

To calculate λ_i for any scattering process in the "could media" model, the collision energy E_{coll} is obtained as follows:

$$E_{coll} = E_{\mu}^{lab}\frac{m_2}{m_1+m_2},$$

where m_1 and m_2 are the masses of the muonic atom and of the media particle respectively, E_{μ}^{lab} stands for the μ-state energy in Laboratory system. Then the reaction rate λ is obtained by spline-interpolation of the first two columns of an appropriate *.fcn file: $\lambda=\lambda(E_{coll})$. The two subroutines VSPLINE and VSPLINT are responsible for all spline interpolation in the code. The first one prepares the interpolation factors, the second one returns the interpolated value.

In the "Hot media" model, λ_i is taken directly from a *.tra file for given $E_{\mu}^{lab} \equiv E_a$ (see section 5.3).

The time interval between two interactions T_{event} is calculated as

$$T_{event} = -\ln\gamma \Big/ \sum_{i=1}^{N_{tr}}\lambda_i .$$

Calculation of new kinematic variables after a transition depends on its class. It is defined by the *.fcn file corresponding to the transition. For example, the class '2->1 0 ' that describes molecular formation, assumes that molecules stop after the reaction. Another class '1->2 W Z', corresponding to atomic capture of muon, provides energy and angle distributions of muonic atoms after the capture.

For scattering processes in the "could media" model, the new kinematics variables of the μ-state after scattering are obtained firstly in the center of mass system (CMS) of the two colliding particles. For this purpose the angular distribution of scattered particles in CMS is used:

$$\frac{d\lambda}{d\cos\theta} = \lambda^{total}\sum_{n=0}^{N-1}C_n(E_{coll})\cos^n\theta ,$$

with coefficients $C_n(E_{coll})$ given in discrete points versus collision energy. For the current (calculated) value of E_{coll} the coefficients $C_n(E_{coll})$ are obtained also by means of spline interpolation. Then the equation

$$\int_{-1}^{1}\sum_{n=0}^{N-1}C_n(E_{coll})\cos^n\theta\, d\cos\theta = \gamma$$

with random number $\gamma \in (0,1)$ is solved to calculate cos θ. The polar scattering angle is uniform: $\varphi=2\pi\gamma$.

Then the energy after the scattering in LAB is

$$E'_a = \frac{m'_a}{2}(V_{CMS}^2 + U_a'^2 + 2V_{CMS}U'_a\cos\theta),$$

where the notation are from the section 5.1, and

$$U'_a = \sqrt{\frac{2E_{fCMS}}{m'_a}}, \quad \vec{V}_{CMS} = \frac{m_a}{m_a+m_b}\vec{V}_a .$$

The new direction of motion is calculated as follows:

$\frac{\vec{V}'_a}{V'_a} = \hat{R}\frac{\vec{V}_a}{V_a}$, where $\hat{R}$ is the rotation matrix that corresponds to the array RV(3,3), see the section 5.3 for details.

The particle energy is determined by the scattering angle, if the target particle is at rest. Simulation in a realistic model of media with moving particles is described in the section 5.2.

When the scattering angle is obtained and the energy after scattering is calculated, the program calculates the velocity vector $\vec{V}$ of the muonic state. The coordinate of the next interaction point is then obtained as

$\vec{r}_{new} = \vec{r}_{old} + \vec{V}T_{event}$, where $\vec{r}_{old}$ is the coordinate of the previous interaction.

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[5] Resonant Formation of dmut Molecules in Deuterium: An Atomic Beam Measurement of Muon Catalyzed dt Fusion, M.C. Fujiwara, A. Adamczak, J.M. Bailey, G.A. Beer, J.L. Beveridge, M.P. Faifman, T.M. Huber, P. Kammel, S.K. Kim, P.E. Knowles, A.R. Kunselman, M. Maier, V.E. Markushin, G.M. Marshall, C.J. Martoff, G.R. Mason, F. Mulhauser, A. Olin, C. Petitjean, T.A. Porcelli, J. Wozniak, and J. Zmeskal, Phys. Rev. Lett. **85**, 1642 (2000). nucl-ex/0008002.