MODELING CREATION OF METHANE AND ITS DERIVATIVES IN THE TOKAMAK EDGE-EFFECT SIMULATION CODE DIVIMP

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ABSTRACT

Cross section and reaction rate coefficients for the creation of Methane (CH_4) and it's derivatives are processed for use in the Monte Carlo simulation code DIVIMP (DIVertor IMPurity). Due to a lack of verifiable experimental data for individual methane fragment reaction cross sections, consideration of hydrocarbons in the plasma solution has been left out of DIVIMP until now. A new module has been developed with utmost flexibility and expandability in mind for integration into DIVIMP. This module follows the state of a hydrocarbon molecule and in a Monte Carlo way, tracks the interactions it undergoes as electrons and protons collide with the fragment. Program structure and development as well as examples of single-step and full-fragment evolution are presented.

ACKNOWLEDGEMENTS

I would like to thank Professor Peter Stangeby for his council and willingness to take me on for a significant project while so far away from Toronto. It's been a long time since I first wrote Prof. Stangeby for information regarding fusion - now that I'm here I know there's no other place I'd rather be.

I would also like to sincerely thank David Elder - DIVIMP and Fortran guru and all around helpful guy. Thanks for your time volunteered to my thesis and keeping me in line to get this module operating. I truly couldn't have accomplished what I did without you.

LIST OF SYMBOLS

E — impact energy (eV)

E_{th} — threshold energy (eV)

$\Delta E_i^{(-)}$ — kinetic energy loss of particle i in a reaction (eV)

$\Delta E_i^{(+)}$ — kinetic energy gain of particle i in a reaction (eV)

$<A>_g$ — quantity A averaged over a finite interval of the parameter g, for g continuous or discrete

T — Maxwellian temperature ($^\circ K$)

v — collisional velocity (m/s)

$\boldsymbol{s}_j$ — cross section of reaction j (cm^2)

$\boldsymbol{s}_{se}$ — semiempirical cross section (cm^2)

$\boldsymbol{s}_{exp}$ — experimental cross section (cm^2)

$\boldsymbol{s}_{ion}$ — ionization cross section (cm^2)

$\boldsymbol{s}_{di}$ — dissociative ionization cross section (cm^2)

$\boldsymbol{s}_{dr}$ — dissociative recombination cross section (cm^2)

$\boldsymbol{s}_i^{tot}$ — total cross section of reaction i (cm^2)

$\boldsymbol{s}_{cx}$ — charge exchange cross section (cm^2)

$\boldsymbol{s}_{ext}$ — empirical extrapolation of cross section (cm^2)

1.0 INTRODUCTION

Transport of hydrocarbon molecules within a tokamak plasma is becoming an increasingly important factor to be considered for mass-transport codes such as DIVIMP (DIVertor IMPurity). Present-day reactors make extensive use of limiters and divertor targets which are in direct contact with the outermost edge of the plasma within the reactor. Often, they are made of graphite, which can readily release carbon atoms and hydrocarbon molecules. In particular, methane and acetylene may be released or sputter from the surface in significant amounts. Currently, only some of the major transport codes have introduced the effect of this type of contamination to the fusion plasma.

Once released into the plasma, hydrocarbon molecules and their fragments can undergo a long list of possible reactions. Each change of state associated with a reaction is characterized by a cross section and thus a probability for occurring within a certain timeframe relevant to the lifetime of the molecule in the plasma. It is this value which is important for modeling each particle transported within the tokamak.

Interactions with other particles are divided into two groups: reactions with electrons and reactions with protons. A methane molecule, for example, will undergo both types of collision with certain probabilities. Once the impact has occurred, though, a variety of reaction products are possible. Most notably, larger molecules may fragment in a variety of ways for different impact energies and collision situations. Also, the distribution of charge on the product molecules usually has more than one possibility.

Take note, though, that any molecule subjected to the temperatures associated with a fusion device is not likely to remain in it's molecular form for long. Methane is a large molecular structure amongst an energetic mixture of energetic ions and electrons. The overall effect of the presence of methane may therefore be small compared to other effects in the core fuel. More and more, however, research is finding that the processes occurring at the edge of the plasma are extremely significant for conditions in the nuclear fusion burning core. Therefore, a method to account for these effects should be implemented to more accurately model the plasma in a tokamak reactor.

2.0 PURPOSE OF THESIS

In order to account for the effects of electron and proton reactions with hydrocarbon molecules, experimental data must be gathered and quantified for analysis. Cross section information for each possible collision must be tabulated and fit to functions of impact energy and target energy, where appropriate. Then, a computer code is required that is able to take this data for relevant conditions in a fusion reactor and apply the effect of hydrocarbon transport and recycling in the plasma. The statistical process must be considered of taking the cross section of a particular reaction and calculating the probability that a single reaction will occur instead of other possibilities. Once we have found the probability of one event over another, we make use of Monte Carlo analysis to decide which possibility of many is deemed to have occurred. Once a single reaction for a single collision event has occurred, we can continue to follow the progress of the product hydrocarbon fragment as it travels through the plasma. In this way, we can track the progress of a methane molecule as hydrogen atoms are stripped away from its structure, eventually leading to a single carbon atom.

This is the goal of this thesis. Using previously compiled analytic fits of experimental data for reaction rate[1], the code developed will be able to make a Monte Carlo estimate of how hydrocarbon molecules and their fragments travel and interact as they encounter energetic electrons and protons in the plasma of a fusion device. Also, integration of this program as a module in the DIVIMP simulation code will be investigated in order to more accurately simulate the plasma conditions near the edge of a tokamak device.

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[1] See reference 1.

3.0 THE CHEMICAL REACTIONS

3.1 METHANE AND IT'S FRAGMENTS

Methane (CH_4) and each of its fragments are listed in Table 1. As shown, each fragment is considered in both it's neutral and single positively charged state, beginning with a positive carbon atom. Successive states represent the addition of a single electron and/or Hydrogen atom.

The state table is set up such that if future additions are desired, they can be done so in consecutively higher state values. This makes representation of states in a hydrocarbon transition code elementary and readily expandable.

State Number	Chemical Representation
1	C^+
2	C
3	CH^+
4	CH
5	CH_2^+
6	CH_2
7	CH_3^+
8	CH_3
9	CH_4^+
10	CH_4

Table 1: Hydrocarbon Fragment State Table

3.2 ELECTRON IMPACT REACTIONS

An energetic electron in the background plasma initiates electron reactions. Cross sections for reaction are highly dependent on plasma temperature (and therefore incident electron energy). Although a dependence on the velocity of the heavier target particle may exist, it may be ignored for fits of cross section with little deviation from the true reaction response.

In many electron impact processes, additional electrons are released as products. Electron energetics, or loss in kinetic energy of incident, $\Delta E_i^{(-)}$, and gain in kinetic energy of product electrons, $\Delta E_i^{(+)}$, are often available where cross section data are listed. Due to the great density of electrons these electrons may be ignored in further analysis.

A threshold electron energy, E_{th}, to initiate the reaction is associated with each interaction. Below this energy, the probability for a reaction is zero. Often this value is interpolated, based on data collected for much higher electron energies and is fit to a polynomial equation.

As an example, take the following electron impact reaction:

$$e + CH_3 \rightarrow CH_3^+ + e + e' \tag{1}$$

Here, an electron of a minimum energy extrapolated to 12.6 eV strikes a CH_3 molecule. The incident electron undergoes a loss of 15 eV and the e' product is found to gain 2 eV after the reaction [2].

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[2] See reference 1, pg. 15.

3.3 PROTON COLLISION REACTIONS

In this case, a hydrogen ion from the plasma interacts with a hydrocarbon molecule or hydrocarbon fragment. Since both particles in this interaction are of similar magnitude in mass, the target particle's velocity can be highly significant. Therefore, for an accurate polynomial description, cross section data should be fit to both the proton energy and the hydrocarbon fragment energy dependence.

Similar to the electron impact data, extrapolation from data for a few data points is commonly made. The authors of reference 1 note that although appropriate interpolation or extrapolation procedures are used, some data may represent only reasonable extensions or theoretical models for particle interaction. See section 5.1 for further discussion of this topic.

4.0 THE COMPUTATIONAL SOLUTION

The computational solution to the hydrocarbon fragmentation calculation involves reading and storing available data for reaction cross sections, and interpreting the data for the required situation in the reactor. As with any programmed solution, there are a number of ways this can be accomplished and programmed. The process followed is described further.

The language chosen to develop the hydrocarbon code is Fortran 90. Although DIVIMP itself is written solely in Fortran 77, there are many features of Fortran 90 which appear attractive for this problem. These include a modular programming approach, derived-type declarations, structured records and dynamic memory allocation. Further explanation of the computational solution is given.

4.1 PROGRAMMING THEORY

As mentioned previously, a great degree of uncertainty may exist in the data available. Therefore, it is advantageous to allow for the maximum amount of future modification and expandability in the code. Polynomial fitted data, for example, may be currently given with a certain order for all reactions allowing for both plasma temperature and target particle energy. In the future though, new, more accurate data may require changes in coefficients. Data are therefore initially read and interpreted when the code is first called from an external database file. In addition, data for new hydrocarbon reactions may become available in the future. Therefore, records are read and stored sequentially from the database until the end is reached. Future data may be found to better fit a polynomial of a different order from that of the existing data. Therefore, arrays of coefficient storage are defined for maximum length of the highest potential polynomial order.

In this way, the hydrocarbon code most easily permits future development.

4.2 DATA AVAILABLE

Data given in the PPPL report used[3] are given in both the $\langle s \rangle$ cross sections and $\langle sv \rangle$ reaction rate coefficients. Reaction rate coefficients are found by integrating the cross section of a particle incident (hydrocarbon fragment) over a Maxwellian distribution of particles (electrons or protons)[4]. These data are fit to polynomials with the following relationships: for cross section data, the logarithm of cross section is fit with equation 2:

$$\ln s = \sum_{n=0}^{N} a_n \left(\ln E \right)^n \tag{2}$$

Reaction rate coefficients for electron reactions are virtually independent of electron energy within the range of energies of importance and are fit similarly with equation 3.

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[3] See reference 1, pgs. 13-69.
[4] For further details, see reference 1, pg. 5.

$$\ln\langle \boldsymbol{s}v\rangle = \sum_{n=0}^{N} b_n \left(\ln T\right)^n \qquad (3)$$

These two equations represent single dependence on either electron energy or plasma temperature for cross section and reaction rate respectively. For the case of proton impact reactions, a double polynomial fit to both energy and temperature is required:

$$\ln\langle \boldsymbol{s}v\rangle = \sum_{n=0}^{N}\sum_{m=0}^{M} a_{mn} \left(\ln E\right)^n \left(\ln T\right)^m \qquad (4)$$

With each fit is an associated error used to indicate the quality of polynomial fit to the experimental data.

$$Error = \frac{1}{N}\sum_{i=1}^{N}\left(\ln x_i - \ln x_{fit,i}\right)^2 \qquad (5)$$

In all cases considered, the fit provided gives an error on the order of 10^{-4} or well within the suggested error of the experimental data.

For both cross section and reaction rate data, 8th order polynomials are fit to the experimental points. This leads to 9 terms required to completely define the polynomial. Graphical representations can be found in Appendix B for both electron and proton reactions.

Take note that in many cases, a steep decline in reaction rate or cross section is found near the threshold energy or temperature. This can be very difficult to fit to and should be considered when using data near or beyond the threshold.

Also of note is that currently the code only supports the use of reaction rate coefficients for probability calculations. This is because utilizing a cross section to find a reaction probability would involve analytic integration which though possible, is highly time consuming. It is suggested for future consideration to take advantage of future reaction profiles whose data is not found in PPPL 2477 but may have been studied since its publish date.

4.3 READING THE DATA

The database file contains all the information given in the PPPL report used as the main source of data. It does so in a record format, each separated by a single space. A sample record is shown below:

```
Reaction:  '3.1.1'
Transition: 10 9
SigmaFT:   1
SigmaVFT:  2
Inputs:    'p+CH4'
Outputs:   'CH4++H'
Datatype:  'Sigma'
Data:     9 3 3
-3.327850106693e+01 -1.608383489195e-01  1.886899005822e-01
-4.166534111130e-02 -1.210872012273e-02  6.257737886111e-03
-9.723353373635e-04  6.518598900821e-05 -1.618150392867e-06
Limits:    1.00e-01 1.01e-14 1.01e-14 9.87e-03
Datatype:  'Sigma-V'
Data:     9 9 9 9
-1.893309642087e+01  1.630850139987e-02 -4.714272469978e-03  2.425492370093e-03  3.068101950239e-03 -1.633878600590e-04 -1.023569804176e-04  1.421483822630e-05 -5.300227927218e-07
 3.776884529381e-01  1.048145245950e-02  7.227733247236e-05 -7.529649417774e-03 -2.850523369529e-04  6.156392408384e-04 -1.035125430666e-04  6.780400601184e-06 -1.596091897574e-07
 1.093763179118e-01 -8.946299454637e-03  5.444574390551e-05  1.707309355637e-03 -4.053883564956e-04 -9.556392408384e-05  3.495664394328e-05 -3.364738102350e-06  1.057092818237e-07
-2.977414700946e-02  6.502084407985e-04  1.092361098382e-03  3.818918718530e-04 -6.507215186222e-05 -2.145885656470e-05  4.842220252995e-06 -3.124588766143e-07  6.085152418331e-09
-3.266919857975e-03  5.754254352327e-04 -4.134810722987e-04 -1.147415418920e-04  7.428734189103e-05 -4.614052740801e-06 -1.313512598842e-06  1.834508345923e-07 -6.495489280153e-09
 2.833761994929e-03 -1.586203199222e-04  2.109974461716e-05  2.696892676495e-06 -1.176543808697e-05  2.542597558870e-06 -7.794570475980e-08 -1.593741872383e-08  9.506440609074e-10
-4.972454353280e-04  1.695706232098e-05  8.410801850446e-06  1.009068906397e-06  2.076254405295e-07 -2.0442160763197e-07  1.818970018754e-08  6.647545290109e-10 -8.054668689989e-11
 3.578860489665e-05 -8.046520550513e-07 -1.200952674126e-06 -6.821482596551e-08  7.011617376997e-08 -4.372775978657e-09  1.989805345252e-10 -8.636301826823e-11  5.648949950364e-12
-9.350695669585e-07  1.323413496981e-08  4.527497936811e-08  7.145677893147e-10 -3.693880360696e-09  6.489051753343e-10 -6.425242445187e-11  5.232989348622e-12 -2.053898151891e-13
Error:    4.76e-04
```

This represents a proton reaction with both cross section and reaction rate polynomials. Descriptions of each identifier in a record can be found at the beginning of the database file (see Appendix A). In general, though, the first six lines give overall details of the particular reaction (PPPL 2477 reaction number, beginning and final states, type of data to come). Then, each record will contain cross section and/or reaction rate data. This will include the number of coefficients for energy or temperature and, if applicable,

target particle dependence polynomials. Also, the number of lines and number of values per line are specified. Then comes the data and finally, error or limit information for the polynomial fit.

Once one record is complete, the loading module moves to the next record until the end of the database file is reached. Comments in the file are allowed if the line begins with a '!' or '#'.

4.4 PROBABILITY CALCULATIONS

Required probability calculations include three functions which must be coded into the hydrocarbon module. First, the probability of an individual reaction given the reaction rate coefficient, plasma density and a time frame for which to consider the reaction possible is found. For this, we use the exponential density function. This relation depends on a single parameter, $l > 0$ and is defined in the form [5]

$$f(x) = \begin{cases} le^{-lx} & x \ge 0 \\ 0 & x < 0 \end{cases},$$
(6)

The cumulative distribution function is found by integrating as follows:

$$F(x) = \int_{-\infty}^{x} f(u)\,du = \begin{cases} 1 - e^{-lx} & x \ge 0 \\ 0 & x < 0 \end{cases},$$
(7)

We can use this relation in the context of a timestep by replacing x with t. The value for l is found by multiplying the plasma density by the interpolated reaction rate as follows:

$$l = r\langle sv \rangle$$
(8)

We can see that this remains dimensionless with a simple analysis.

$$r = \left[\frac{1}{cm^3} \right]$$
(9a)

$$\langle sv \rangle = \left[cm^2 \cdot \frac{cm}{s} \right] = \left[\frac{cm^3}{s} \right]$$
(9b)

$$lt = \left[\frac{cm^3}{s} \right] \cdot \left[\frac{1}{cm^3} \right] \cdot [s]$$
(9c)

Which is dimensionless.

Next, the total probability for a transition given a number of possible modes of transition will be required. Independently, each reaction process will lead to a transition with a given probability (potentially up to 1.0). We must find the sum of probabilities by any process possible. This is accomplished with the following relationship[6]

$$P(R_1 \cap R_2 \cap ... \cap R_n) = (1 - P_{R_1})(1 - P_{R_2})...(1 - P_{R_n})$$
(10)

This will give the probability of no reaction (the only common possibility among different possible transitions is the lack of a transition. The probability for a reaction is then

$$P(R) = 1 - P(R_1 \cap R_2 \cap ... \cap R_n)$$
(11)

And finally, from the given reaction probabilities, we must be able to find the probability of each reaction occurring given that a reaction does happen. For this we simply normalize each probability for reaction by the sum of individual probabilities.

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[5] See reference 3, pg.48-49.
[6] See reference 4, pg 23.

$$P(R_i) = P(R_i) / \sum_{i=1}^{n} P(R_i) \qquad (12)$$

4.5 THE MONTE CARLO APPROACH

Monte Carlo analysis is performed with the aide of a random number generator (RNG). The RNG is seeded or given an initial value to begin it's random number algorithm and returns a value randomly but evenly distributed over a range of 0 to 1. Because this process depends on an initial seed, the value returned is not truly random but pseudorandom. What this means is that after seeding the RNG with the same value, the same random values will be returned in succession. For our purposes, though, this is sufficient. Future expansion and integration into DIVIMP may require a more sophisticated RNG.

Given a series of reactions and the question of whether a single reaction occurs is a situation where an RNG could be used. The random value drawn from the RNG could be compared to the total probability of any single reaction given the set of possibilities: if less than the total probability, a reaction occurs. If the random value is higher that the total probability, we move ahead a timestep and check again to see if a reaction occurs.

If we find that a reaction among a set of reactions does occur, another random value can be drawn to decide which reaction has taken place. The random value is compared to a set of probabilities calculated in an additive way to see where the random number lies and therefore which reaction takes place. For example, if we have the following normalized probabilities for different possible reactions:

$$P(R_1, R_2, R_3) = \{0.25, 0.50, 0.25\} \qquad (13)$$

We convert the probabilities to an additive set as shown:

$$P(R_{1a}) = 0.25 \text{ (no change)} \qquad (14a)$$

$$P(R_{2a}) = 0.50 + P(R_{1a}) = 0.50 + 0.25 = 0.75 \qquad (14b)$$

$$P(R_{3a}) = 0.25 + P(R_{2a}) = 0.25 + 0.75 = 1.00 \qquad (14c)$$

$$P(R_{1a}, R_{2a}, R_{3a}) = P_a(R) = \{0.25, 0.75, 1.00\} \qquad (14d)$$

Thus, a random value between 0 and 1 can now be selected and compared to the range for individual reaction probability. In this way, a final state given a reaction occurring from a number of reactions can be found.

5.0 Programming the Code

5.1 PLATFORM INFORMATION

As previously stated, the hydrocarbon module code was programmed in Fortran 90. This was accomplished on two platforms. First, initial testing was done on Compaq Visual Fortran (CVF) 5.0 under a Windows 98 operating system on a Pentium 233 platform. Further along in the development, the code was transferred to a Redhat Linux 6.0 OS under the same platform. The purpose of this was to process the code under the same compiler as DIVIMP, PGI Fortran 3.0 (The Portland Group, Inc.), and then later on to version 3.1.

Noteworthy differences between the two compilers are as follows:

-No 'EOF' (End Of File) use ability in PGI Fortran. Instead, use the IO_RESULT return value from a read statement to determine if you have reached the last line of an input file.

-Differences in the random number generator. In CVF, the RNG is seeded with a value determined from the date and time.

5.2 PROGRAM STRUCTURE

The hydrocarbon module is organized in the manner presented in Figure 1. A wrap-around program, HC_Demo does the job of loading the main database from the external data file and successively calling the

main function, HC_NewSt. Here, the new state(s) is found with the aid of modules containing both probability and statistical procedures. HC_Demo has it's own data file, HC_Demo.dat, which it accesses to learn reactor conditions for the test and the initial hydrocarbon state. The main data file is loaded after first defining data structures (see 5.4) with HC_Setup, and initializing them to inceptive values (commonly '0's). HC_LdDta then opens the database file to read in all required information into the structures setup. In order to allow other modules to access these structures when required, the Fortran 'Use' statement is called at the beginning of the module in question. In this way, for example, HC_RnPrb can enter the storage area for reaction rate coefficients and calculate the reaction probability required. From HC_NewSt, HC_RnLup is called to find which states are immediately accessible by a single reaction from the current state, HC_RnPrb is called to find the associated probabilities, HC_TlPrb is called to find the total probability for transition and HC_NSPrb is called to find the normalized state transition. If the case specified is an informative one, the process is complete. If it is a statistical evolution case, the program begins by calling the random number generator, HC_RNGen, to see if a change of state occurs. If so, another call to HC_RNGen gives the new state and the processes repeats itself as specified previously.

All output is handled by HC_Demo. An output file is created which contains the data put on the screen throughout the run(s) called in the HC_Demo.dat file. When complete, this is put in the user directory where the code was originally called.
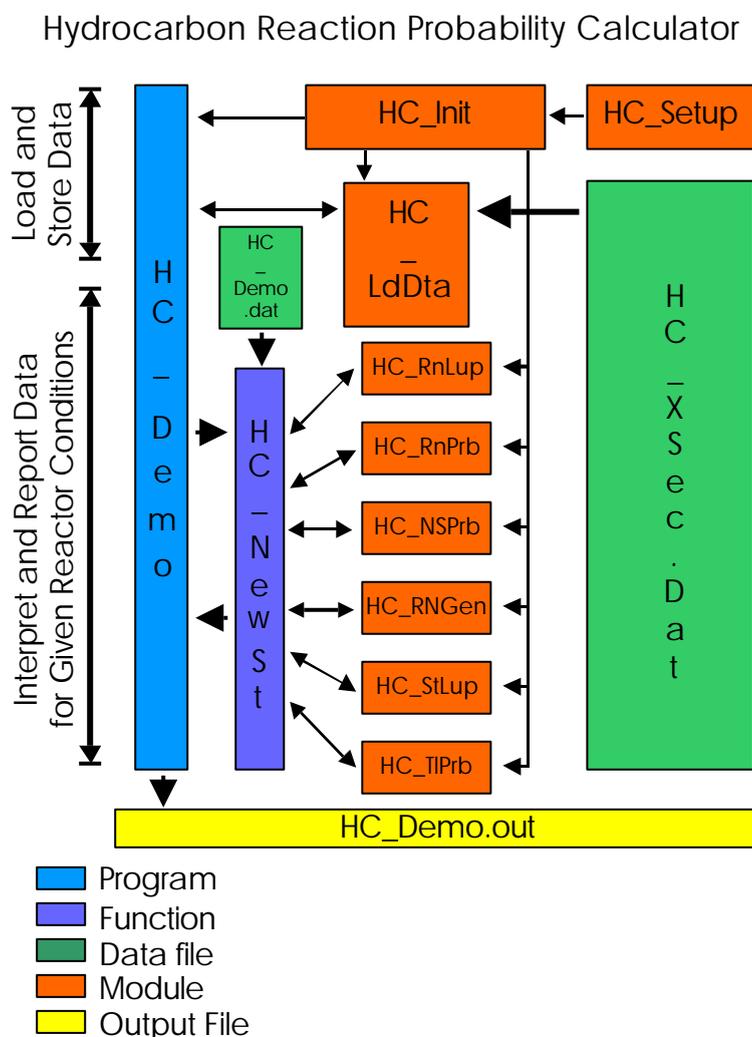

Figure 1: Program Flow Diagram

5.3 DATA STORAGE

Data are stored in five main tables. The first shown previously on page 7, table 1, is the State Table. This array assigns values to each state from a positively charged Carbon atom up to (currently) a neutral Methane molecule and is defined by a maximum number of states variable which must be set by the user. This table is used for program simplicity but also used for output clarity.

The second table is referred to as the Reaction Table. This two-dimensional array contains each defined state and the number of reactions which take that state and transform it to another. Then, it contains the reaction numbers of each affecting transition. This table is defined by a preset maximum number of reactions variable that must be changed by the user if more reactions are added.

State Number	Number of Reactions Affecting	Reaction	Reaction	Reaction
1	0	0	0	0
4	3	2	1	1
10	2	8	5	0

Table 2: Reaction Table

The third table is the State Transform Table. This two-dimensional array is fed specific information about each reaction as it is read in from the main database. It contains the reaction number (defined on the fly as each reaction is read in from the data file), the initial and final states associated with each reaction (determined from the State Table), whether the reaction involves an electron or proton, and information about the way cross section and reaction rate polynomials are stored. First, whether the fits are dependent solely on plasma temperature (a value of 1) or defined as both temperature and target particle dependent (a value of 2) is stated. Then, the number of coefficients in the polynomial for cross section and reaction rate is found.

Reaction Number	Initial State	Final State	Electron or Proton Reaction	Sigma Target Particle Dependence	Sigma Polynomial Order - 1	SigmaV Target Particle Dependence	SigmaV Polynomial Order - 1
10	9	8	'e'	1	9	1	9
25	3	2	'e'	1	9	1	9
30	4	1	'p'	1	9	2	9

Table 3: State Transform Table

The purpose of the final two tables is to store coefficient values for the definition of cross section and reaction rate polynomials. These are called Sigma_Data (for cross sections) and SigmaV_Data (for reaction rates). In contrast to the other tables, these arrays are three-dimensional. This allows each set of data to be fully defined with both temperature and target energy dependence (i.e. 9x9 array of coefficients for each reaction polynomial definition. To visualize this data structure, view Figure 2. In it we see how the ith reaction is defined with j terms in the temperature dependent polynomial and k terms in the target particle dependent polynomial definition.
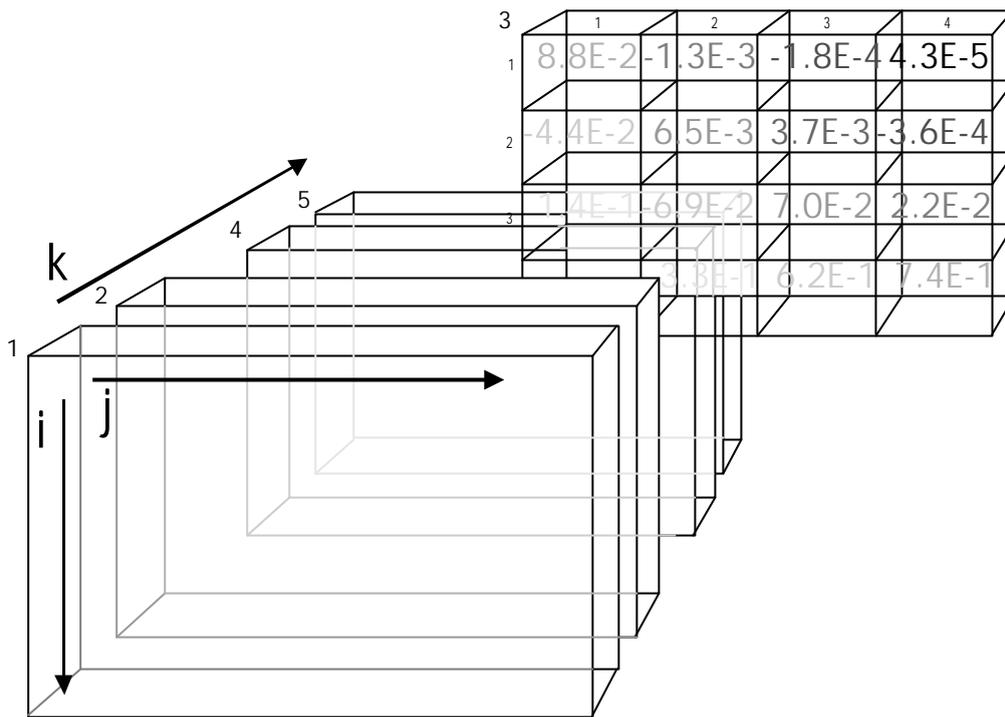
Figure 2: 3-Dimensional Polynomial Coefficent Storage

With the data in PPPL 2477, we can see there will be little use of the capabilities of this data structure. Although it allows for all electron and proton reactions and each cross section and reaction rate definition to be defined with colliding and target particle energy and as variables, only the proton Sigma-V data contains a full data set. Each of the other sets of data have only colliding particle dependence for both Sigma and Sigma-V data.

6.0 Using The Program

6.1 INFORMATION MODE

If data is requested for the probability of transition from a given current state to each of the possible transition states given the current reaction database, the *information mode* is used. In this mode, the code looks through the state transform table for an initial state equal to the current state as given. It then fills an array (of length of a preset maximum number of possible transitions) with possible transitions. For each possible transition, a reaction probability, and a normalized probability are calculated as previously described. Also, a total probability for transition is found and reported. Output is formatted for easy readability and both printed to the screen and saved to a file in the current directory.

6.2 MONTE CARLO MODE

If the user would like to see how a single hydrocarbon fragment evolves until the fragment becomes a carbon atom (without a hydrogen component), a full listing Monte Carlo analysis is selected. For a given current state in the existing state table, the same analysis as above is carried out transparently (no output is printed). Then, a single random number is drawn to determine if a change of state takes place. If the random value is larger than the total probability for a reaction, no reaction takes place and a counter is incremented to indicate that one timestep has gone by without a reaction. If a reaction is indicated (random number < total probability), then another random value is drawn to decide which final state of the possible

reactions we end up in. The normalized probabilities are calculated in an additive way (see section 4.5) and compared to the random value until the random number is no longer larger than the additive normalized probability. In mathematical terms:

$$P_a(R_n) < RN < P_a(R_{n+1}) \tag{15}$$

with

$$P_a(R_n) \geq 0, P_a(R_{n+1}) \leq 1$$

Once the new state has been decided upon, a check is made to see if the final state (a positively charged carbon ion) has been reached. If not, the process repeats, this time with the current state being the hydrocarbon fragment product of the previous reaction. Again, output is printed in a easily read format and saved to a file on the disk.

6.3 ADDING A RECORD

The procedure to add a record in the reaction database file has been made as effortless as possible. If the new reaction does not contain a hydrocarbon fragment not in the current state table, adding a new reaction is as simple as extending the reaction file in the same format as any current record. Both $\langle s \rangle$ and $\langle sv \rangle$ data may be represented as to plasma temperature and target energy dependence, each defined by a polynomial of variable order.

If a reaction to be added contains a hydrocarbon not listed in the current state table, it may be added. Be careful to attempt to consider all possible reactions for a hydrocarbon fragment if desired output is to be analyzed for transitions to a final carbon state. If a complete definition for state transition is not listed, the Monte Carlo analysis will not be accurate for reactor relevant conditions.

7.0 Results

7.1 SINGLE TRANSITION INFORMATIVE RUNS

For this case, the probabilities are listed for all possible transitions given the current reaction library. This is accomplished by a search through the reaction table for the specified state and making a list of possible reactions involving that state. The probability for each possible transition is then calculated given the plasma temperature and potentially target energy, plasma density, the timestep for reaction and the interpolated $\langle s \rangle$ or $\langle sv \rangle$ value. The code then normalizes each value of individual probabilities by the total. A sample information run is printed below:

```
Case Data                25
Run Type                 Info
Data Type:               SigmaV
Current_State:           9    CH4+
Plasma Density:          0.100E+15
Plasma Temperature:      0.100E+02
Target Energy:           0.1E+00
Hydrogen Mass:           0.1E+01
Timestep:                0.100E-07
Destination Reaction Iden. Reaction Type Reaction Prob. Normalized Prob.
  8   CH3     '2.15.1'         e           0.699 %          13.671 %
  7   CH3+    '2.15.2'         e           2.084 %          40.729 %
  8   CH3     '2.19.1'         e           0.132 %           2.572 %
  6   CH2     '2.19.2'         e           0.394 %           7.705 %
  3   CH+     '3.1.4'          p           1.807 %          35.324 %
Total Probability for state change    5.027 %
```

Shown is the transition table for a CH_4^+ ion at a hydrogen plasma electron density of 10^{14} $1/cm^3$ and a temperature of 10 eV in a timestep of 10^{-8} s. Five possible destination states are found in the current state

transform table (via four electron and 1 proton reaction) and each reaction probability is reported based on the interpolated reaction cross section.

As an example, for e+CH -> C+H+e (reaction 2.14), the interpolated reaction rate based on the Sigma-V data is given by:

$$\langle \boldsymbol{s}v \rangle = \exp\left(\sum_{n=0}^{8} b_n \left(\ln T \right)^n \right) \tag{16a}$$

$$= \exp\left[\begin{array}{l} \left(-2.94e+01\right)\left(\ln 10\right)^0 + \left(1.11e+01\right)\left(\ln 10\right)^1 + \left(-4.96e+00\right)\left(\ln 10\right)^2 \\ + \left(1.39E+00\right)\left(\ln 10\right)^3 + \left(-2.57e-01\right)\left(\ln 10\right)^4 + \left(3.12e-02\right)\left(\ln 10\right)^5 \\ + \left(-2.40e-03\right)\left(\ln 10\right)^6 + \left(1.05e-04\right)\left(\ln 10\right)^7 + \left(-2.00e-06\right)\left(\ln 10\right)^8 \end{array} \right] \tag{16b}$$

$$= 7.58e-09 \text{ cm}^3/\text{s} \tag{16c}$$

The reaction probability is found from:

$$P\left(R_1\right) = 1 - e^{-1t} = 1 - e^{-(7.58e-09 \cdot 1e14) \cdot 1e-8} = 0.007 \tag{17}$$

For the total probability, we have:

$$P_T\left(R_n\right) = 1 - \left(1-0.007\right)\left(1-0.021\right)\left(1-0.001\right)\left(1-0.004\right)\left(1-0.018\right) = 0.050 \tag{18}$$

For the first normalized probability, we have:

$$P_{NS}\left(R_1\right) = \frac{0.00699}{\left(0.007 + 0.021 + 0.001 + 0.004 + 0. - 18\right)} = 0.137 \tag{19}$$

Sample data are shown for 3 examples of reactor-relevant conditions for each of the current 10 possible states in Appendix D.2.

7.2 FULL TRANSITION TO SINGLE CARBON STATE

When a full transition case is selected, the same procedure for statistical analysis for a single transition is done. Once possible transition states are found with associated probabilities, a random number is drawn to see if a transition occurs. If a transition is indicated, another random value is drawn to select which possible state the current state moves to. This process is continued until the fragment is reduced to a carbon particle. When a possible transition in a timestep does not translate into a change of state, a counter is incremented. This value, the number of timesteps before a transition, is reported along with each transition selected in a Monte Carlo way and the random value drawn.

An example is shown for a CH hydrocarbon fragment injected into a plasma of density 10^{14} cm^{-3}, temperature 10 eV with a timestep of 10^{-8} s:

```
Case Data                34
Run Type                 Stat
Data Type:               SigmaV
Current_State:           4    CH
Plasma Density:          0.100E+15
Plasma Temperature:      0.100E+02
Target Energy:           0.1E+00
Hydrogen Mass:           0.1E+01
Timestep:                0.100E-07
   Start      Next    Reaction Iden. Timesteps Total Prob. Random Number
   4   CH    3   CH+      '3.1.4'        36       3.968 %    0.0354708
   3   CH+   2   C        '2.22'        108       1.396 %    0.0086230
   2   C     1   C+       '2.23'         51       2.933 %    0.0031198
```

Evolution through successively simpler hydrocarbon is clearly demonstrated, as is the use of Monte Carlo selection.

Sample data can be found in Appendix D.3 for 17 different initial conditions.

8.0 The Future

The hydrocarbon module is not yet integrated into DIVIMP. For use in the main code, DIVIMP requires only change of state information to be returned from a hydrocarbon molecule incident on the plasma. For this, product particles must be categorized as either neutral or charged. This is so that, when injected into the DIVIMP reactor edge model, the effect of magnetic confinement can effect the charged particles and neutrals can cross magnetic fields without effect. The code for transport of these states exist although they are not mass dependent up to the potential magnitude of transport of a methane molecule (i.e. a carbon of mass 12 amu).

To facilitate this data exchange, the hydrocarbon code was written as a main program (HC_Demo.f90) interacting with the module to calculate transition state probabilities. For use in DIVIMP, the HC_Demo main program would be discarded and DIVIMP would interact with HC_NewSt directly. Also, with this configuration, the effect of varying reactor conditions from timestep to timestep can be accounted for. This is necessary for a true plasma simulation.

9.0 Conclusions

A module to load, and interpret hydrocarbon transition probabilities was written and demonstrated. A complete format for data storage and retrieval was developed and proven to operate effectively for use in both basic informative calculations and Monte Carlo state evolution through available hydrocarbon reactions.

There is a clear future for this work. This is but a computational engine for the code necessary to facilitate hydrocarbon transport in DIVIMP. The bridge to this goal is one which is in sight and in our grasp. I would encourage future development based on this design and hope to one day see it working in concert with the DIVIMP code.

10.0 REFERENCES

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2. <u>Ibid</u>.
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4. <u>Ibid</u>.
5. <u>Ibid</u>.

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Appendix A: Sample Contents of Hydrocarbon Reaction Data File

```
! DIVIMP HydroCarbon Module Data File
! Adam McLean under Prof. Peter Stangeby
! Resarch engineer: David Elder
! October, 1999
!
! This file contains all polynomial values for complete descriptions
! of the cross section and reaction rate data for carbon reactions
! occurring in a plasma of variable background plasma temperature (T)
! and target particle energy (E).
!
! Data is expected in the following format:
! a) Reaction:      Reaction number from PPPL-2477
!                   Character*10 in single quotes
! b) Transition:    Call table for initial state to final state
!                   Two intgers*3 separated by a single space
! c) SigmaFT:       Target Particle dependence fit data (1) or independent data (2) for Sigma data
!                   Optional if SigmaVFT is defined
!                   Integer*1
! d) SigmaVFT:      Target Particle dependence fit data (1) or independent data (2) for SigmaV data
!                   Optional if SigmaFT is defined
!                   Integer*1
! e) Inputs: Electron or proton plus hydrocarbon
!                   Character*10 in single quotes
! f) Outputs:       Reaction products
!                   Character*10 in single quotes
! g) Datatype:      Sigma cross section or Sigma-V reaction rate
!                   Character*10 in single quotes
! h) Data:  Number of terms in temperature dependence polynomial - poly nomial order + 1
!           followed by number of lines of data and coefficients per line
!           followed by terms in target particle energy dependence polynomial if applicable
!           3 x Integer*3 [3 x Integer*3] each separated by a single space
!           Data is expected in the following form:
!           Background temperature dependence: 3 lines each of 3 real values
!           Background and target particle dependence: 9 lines each of 9 real values
! f) Limits: Data for fit applicability expected in the following form:
!           Background temperature dependence only: Minimum energy for applicability
!           Sigma/SigmaV at minimum energy/temp
!           Maximum applicable Sigma/SigmaV
!           Error associated with fit
!           All values Real separated by single spaces
! g) Error:  Error associated with target particle plus background temperature dependent fit
!           Real
!
! Assumptions for Data:
! 1) For target particle independent data, energy of target particle is considered to be zero.
! 2) Sigma fits are valid for 0.1 < E < 2000eV.
!
! Notes:
!      Only one of Sigma or SigmaV data sets are required in each reaction data set.
!   Whether each is available is determined by the definition of the SigmaFT and SigmaVFT values.
!   If the data provided does not correspond to the selected data in the test data file,
!   an error is reported.
! Fits for Sigma and Sigma-V for electron interactions

Reaction:  '2.1'
Transition: 10 9
SigmaFT:   1
SigmaVFT:  1
Inputs:    'e+CH4'
Outputs:   'CH4++2e'
Datatype:  'Sigma'
Data:      9 3 3
-1.692667783851e+03  2.361715778264e+03  -1.438324660013e+03
 4.887024369590e+02 -1.013809397590e+02   1.316222364453e+01
-1.045724814875e+00  4.654403722971e-02  -8.896748338271e-04
Limits:    1.43e+01 1.00e-19 1.80e-16 2.39e-01
Datatype:  'Sigma-V'
Data:      9 3 3
-3.130271609338e+01  1.296168986190e+01  -5.500277167544e+00
 1.468759127748e+00 -2.515405069844e-01   2.710024229192e-02
-1.786606299569e-03  6.605572407734e-05  -1.051047534357e-06
Limits:    1.58e+00 3.52e-12 1.04e-07 3.54e-06

Reaction:  '3.1.1'
Transition: 10 9
SigmaFT:   1
SigmaVFT:  2
Inputs:    'p+CH4'
Outputs:   'CH4++H'
Datatype:  'Sigma'
Data:      9 3 3
-3.327850106693e+01 -1.608383489195e-01   1.886899005822e-01
-4.166534111130e-02 -1.210872012273e-02   6.257737886111e-03
-9.723353373635e-04  6.518598900821e-05  -1.618150392867e-06
Limits:    1.00e-01 1.01e-14 1.01e-14 9.87e-03
Datatype:  'Sigma-V'
Data:      9 9 9 9
-1.893309642087e+01  1.630850139987e-02 -4.714272469978e-03  2.425492370093e-03  3.068101950239e-03 -1.633878600590e-04 -1.023569804176e-04  1.421483822630e-05 -5.300227927218e-07
 3.776884529381e-01  1.048145245950e-02  7.227733247236e-03 -7.529649417774e-03 -2.850523369529e-04  6.156392408384e-04 -1.035125430666e-04  6.780400601184e-06 -1.596091897574e-07
 1.093763179118e-01 -8.946299454637e-03  5.444574390551e-05  1.707309355637e-03 -4.053883564956e-04 -9.556392408384e-05  3.495664394328e-05 -3.364738102350e-06  1.057092818237e-07
-2.977414700946e-02  6.502084407985e-04  1.092361098382e-03  3.818918718530e-04 -6.507215186222e-05 -2.145885656470e-05  4.842220252995e-06 -3.124588766143e-07  6.085152418331e-09
-3.266919857975e-03  5.754254353327e-04 -4.134810722987e-04 -1.147415418920e-04  7.428734189103e-05 -4.614052740801e-06 -1.313512598842e-06  1.834508345923e-07 -6.495489280153e-09
 2.833761994929e-03 -1.586203199222e-03  2.109974461716e-05  2.696892676495e-06 -1.176543808697e-05  2.542597555870e-06 -7.794570475980e-08 -1.593741872383e-08  9.506440609074e-10
-4.972454353280e-04  1.695706232098e-05  8.410801850446e-06  1.009068906397e-06  2.076254405295e-07 -2.044216076319e-07  1.818970018754e-08  6.647545290109e-10 -8.054668689989e-11
 3.578860489665e-05 -8.046520550513e-07 -1.200952674126e-06 -6.821482596551e-08  7.011617376997e-08 -4.372775978657e-09  1.989805345252e-10 -8.636301826823e-11  5.648949950364e-12
-9.350695669585e-07  1.323413496981e-08  4.527497936811e-08  7.145677893147e-10 -3.693880360696e-09  6.489051753343e-10 -6.425242445187e-11  5.232989348622e-12 -2.053898151891e-13
Error:     4.76e-04
```

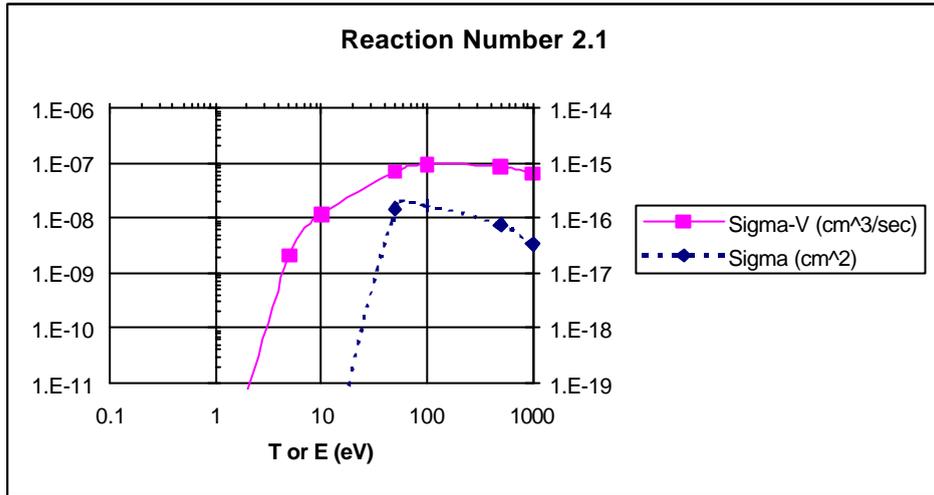Appendix B: Sample Graphical Reaction Cross Section Data

Figure 3: e + CH$_4$ -> CH$_4^+$ + 2e

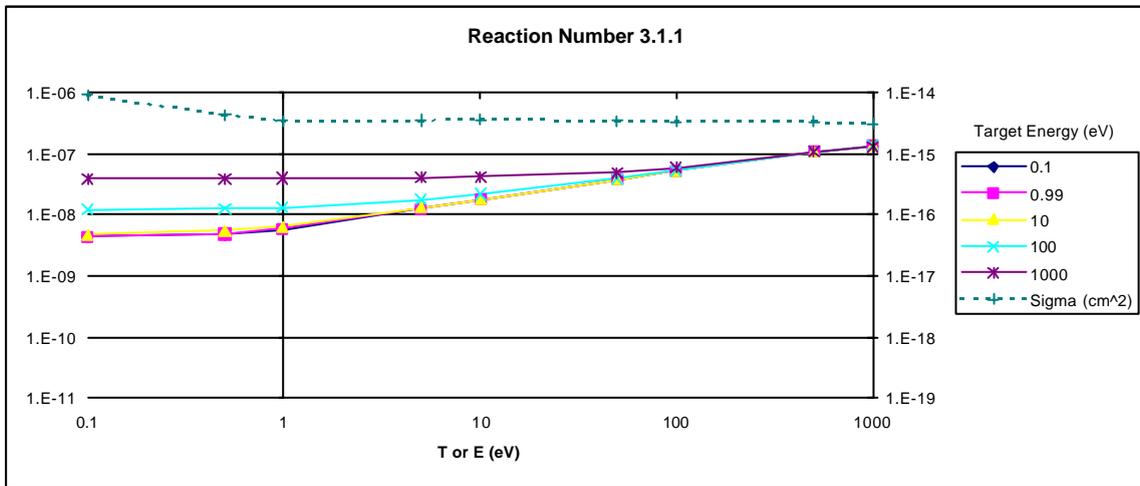**Figure 4: p + CH$_4$ -> CH$_4^+$ + H**

Appendix C: HC_Demo.dat Data File for Sample Results Output

```
! Sample Data file for example probability calculations

! Data in the form
run_type,current_state,density,temperature,target_energy,hydrogen_mass,output_flag,timestep
! Options
!  (1) run_type     - 'Info' - give probability and state data for a single transition
!                   - 'Stat' - give all steps from current to final transition
!  (2) data_type    - 'Sigma' - sigma data used from data file
!                   - 'SigmaV' - sigma-V data used from data file
!  (3) current_state - initial state number (#)
!  (4) density        - background plasma density (particles/cm^3)
!  (5) temperature   - background plasma temperature (eV)
!  (6) target_energy - target particle energy (eV)
!  (7) hydrogen_mass - indicates a deuterium (1) or tritium (2) plasma
!  (8) output_flag   - 'Off' - turns probability and current state data off
!                   - 'On' - turns probability and current state data on
!  (9) timestep      - time step value used in probability calculation (s)

! (1)      (2)  (3)  (4)   (5)(6)(7)(8)(9)

'Info' 'SigmaV' 1  1e14 1e1 0.1 1 'On'  1e-8
'Info' 'SigmaV' 1  1e13 1e1 0.1 1 'On'  1e-8
'Info' 'SigmaV' 1  1e14 1e2 0.1 1 'On'  1e-9
```

Appendix D: Results for Single-Step Cases

```
Case Data                  1
Run Type                   Info
Data Type:                 SigmaV
Current_State:             1   C+
Plasma Density:            0.100E+15
Plasma Temperature:        0.100E+02
Target Energy:             0.1E+00
Hydrogen Mass:             0.1E+01
Timestep:                  0.100E-07
Destination Reaction Iden. Reaction Type Reaction Prob. Normalized
Prob.
Total Probability for state change   0.000 %


Case Data                  40
Run Type                   Stat
Data Type:                 SigmaV
Current_State:             9   CH4+
Plasma Density:            0.100E+15
Plasma Temperature:        0.100E+02
Target Energy:             0.1E+03
Hydrogen Mass:             0.1E+01
Timestep:                  0.100E-07
   Start      Next      Reaction Iden. Timesteps Total Prob. Random
Number
  9 CH4+  8  CH3    '2.15.1'          17      3.279 %   0.0170581
  8 CH3   6  CH2    '2.12'             9      5.947 %   0.0302799
  6 CH2   3  CH+    '2.9'             15      5.085 %   0.0202838
  3 CH+   2  C      '2.22'           176      1.396 %   0.0096696
  2 C     1  C+     '2.23'            46      2.947 %   0.0010569
```