Analysis of an Improved Fusion Reaction Rate Model for Use in Fusion Plasma Simulations

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ABSTRACT

An analysis of reaction rate models from the NRL Plasma Formulary, BUCKY 1-D radiation hydrodynamics code and DRACO 2-D radiation hydrodynamics code are compared to the reaction rate model developed by H. S. Bosch and G. M. Hale. The reaction rates for $T(d,n)^4He$, $D(d,n)^3He$, D(d,p)T and $^3He(D,p)^4He$ fusion reactions were analyzed. A timing analysis was performed to compare computation times of the BUCKY and Bosch-Hale models. It was found that the Bosch-Hale reaction rate equations gave more accurate results at low plasma energies while increasing computational cost by 1% over the reaction rate equation used in BUCKY.

Introduction

Most modern computer simulations of fusion reaction rates utilize fitting functions based on reaction rates calculated from data that was published almost thirty years ago [1]. During the course of the last thirty years, improved experimental techniques were developed that allowed for the collection of more accurate data at low plasma temperatures [2].

This paper analyzes the new reaction rate model proposed by H. S. Bosch and G. M. Hale [2] and compares their R-matrix reaction rate model with the published values found in the Naval Research Laboratory (NRL) Plasma Formulary [3], the BUCKY 1-D radiation hydrodynamics code developed at the University of Wisconsin – Madison [4] and the DRACO 2-D radiation hydrodynamics code developed at the Laboratory for Laser Energetics (LLE) [5].

NRL Plasma Formulary Reactivity

In order to provide a baseline comparison, the reaction rate data for the $T(d,n)^4He$, $D(d,n)^3He$ + D(d,p)T (DD_{total}), and $^3He(D,p)^4He$ fusion reactions from the NRL Plasma Formulary [3] is included in Table 1. This published set of values is based on data from Duane [6].

Temperature (keV)	$T(d,n)^4He$ (cm^3/s)	DD_{total} (cm^3/s)	$^3He(D,p)^4He$ (cm^3/s)
1	5.50E-21	1.50E-22	1.00E-26
2	2.60E-19	5.40E-21	1.40E-23
5	1.30E-17	1.80E-19	6.70E-21
10	1.10E-16	1.20E-18	2.30E-19
20	4.20E-16	5.20E-18	3.80E-18
50	8.70E-16	2.10E-17	5.40E-17
100	8.50E-16	4.50E-17	1.60E-16

Table 1. *NRL Plasma Formulary Reaction Rate Data*

DRACO Reactivity

DRACO is a two-dimensional radiation hydrodynamics code developed by LLE to simulate experiments performed on the OMEGA laser [5]. The reaction rate subroutine uses tabulated data from Hively (1977) [1]. Table 2 contains a subset of the tabulated data found in the DRACO reaction rate subroutine.

BUCKY Reactivity

BUCKY is a one-dimensional radiation hydrodynamics code developed by the University of Wisconsin that models high energy density fusion plasmas [4]. The fusion reaction rate subroutine uses an exponential data fitting function to generate fusion reactivities as a function of plasma thermal energy,

$$\langle \sigma v \rangle = \exp\left[\frac{A_1}{T^r} + A_2 + A_3 T + A_4 T^2 + A_5 T^3 + A_6 T^4 \right] \quad . \tag{1}$$

The coefficients for equation (1) as given in the BUCKY source code are given in Table 3. Table 4 shows the fusion reaction rates resulting from this equation for each of the fusion reaction species.

Temperature (keV)	$T(d,n)^4He$ (cm^3/s)	$D(d,n)^3He$ (cm^3/s)	D(d,p)T (cm^3/s)	DD_{total} (cm^3/s)	$^3He(D,p)^4He$ (cm^3/s)
1	5.48E-21	6.92E-23	8.30E-23	1.52E-22	3.02E-26
2	2.62E-19	2.60E-21	2.82E-21	5.42E-21	1.42E-23
5	1.30E-17	8.94E-20	8.78E-20	1.77E-19	6.65E-21
10	1.08E-16	6.26E-19	5.81E-19	1.21E-18	2.28E-19
20	4.28E-16	2.73E-18	2.43E-18	5.16E-18	3.79E-18
50	8.64E-16	1.11E-17	9.66E-18	2.08E-17	5.46E-17
100	8.50E-16	2.51E-17	2.13E-17	4.64E-17	1.60E-16

Table 2. *DRACO Reaction Rate Data.*

	$T(d,n)^4He$	DD_{total}	$^3He(D,p)^4He$
A_1	-2.1377692E+01	-1.5511891E+01	-2.7764468E+01
A_2	-2.5204050E+01	-3.5318711E+01	-3.1023898E+01
A_3	-7.1013427E-02	1.2904737E-02	2.7889999E-02
A_4	1.9375450E-04	2.6797766E-04	-5.5321633E-04
A_5	4.9246592E-06	-2.9198658E-06	3.0293927E-06
A_6	-3.9836572E-08	1.2748415E-08	-2.5233325E-08
r	0.2935	0.3735	0.3597

Table 3. *Coefficients used in the reaction rate polynomial for BUCKY.*

Temperature (keV)	$T(d,n)^4He$ (cm^3/s)	DD_{total} (cm^3/s)	$^3He(D,p)^4He$ (cm^3/s)
1	5.48E-21	8.52E-23	3.02E-26
2	2.62E-19	2.97E-21	1.42E-23
5	1.30E-17	9.98E-20	6.65E-21
10	1.08E-16	7.53E-19	2.28E-19
20	4.28E-16	4.08E-18	3.79E-18
50	8.64E-16	3.51E-17	5.46E-17
100	6.56E-16	2.92E-16	1.74E-16

Table 4. *Reaction Rate Data based on the polynomial equation used for BUCKY.*

Bosch-Hale Reactivity

R-matrix theory [7] [8] was used by Bosch and Hale [2] in conjunction with more recent low-energy experimental cross section data [9] [10] [11] to derive a more accurate fusion reactivity model. Equations (2) through (5) are the result of the R-matrix fit to the experimental data. For the fusion reactions described in this paper, Bosch and Hale compare their R-matrix fit to experimental data (Appendix I, Fig. 2-15).

$$B_G = \pi\alpha Z_1 Z_2 \sqrt{2 m_r c^2} \tag{2}$$

$$\theta = T \Bigg/ \left[1 - \frac{T\left(C_2 + T\left(C_4 + TC_6\right)\right)}{1 + T\left(C_3 + T\left(C_5 + TC_7\right)\right)} \right] \tag{3}$$

$$\xi = \left(\frac{B_G^2}{4\theta} \right)^{1/3} \tag{4}$$

$$\langle \sigma v \rangle = C_1 \theta e^{-3\xi} \sqrt{\xi / \left(m_r c^2 T^3 \right)} \tag{5}$$

Table 5 shows the coefficients used by Bosch and Hale in the equations above. Table 6 shows the fusion reactivities calculated from the Bosch-Hale model.

	$T(d,n)^4He$	$D(d,n)^3He$	D(d,p)T	$^3He(D,p)^4He$
C_1	1.17E-09	5.43E-12	5.66E-12	5.51E-10
C_2	1.51E-02	5.86E-03	3.41E-03	6.42E-03
C_3	7.52E-02	7.68E-03	1.99E-03	-2.03E-03
C_4	4.61E-03	0.00E+00	0.00E+00	-1.91E-05
C_5	1.35E-02	-2.96E-06	1.05E-05	1.36E-04
C_6	-1.07E-04	0.00E+00	0.00E+00	0.00E+00
C_7	1.37E-05	0.00E+00	0.00E+00	0.00E+00
m_rc^2 (keV)	1124656	937814	937814	1124572

Table 5. *Coefficients used in the equations for determining the reaction rate by the Bosch-Hale method.*

Temperature (keV)	$T(d,n)^4He$ (cm^3/s)	$D(d,n)^3He$ (cm^3/s)	D(d,p)T (cm^3/s)	DD_{total} (cm^3/s)	$^3He(D,p)^4He$ (cm^3/s)
1	6.86E-21	9.93E-23	1.02E-22	2.01E-22	3.05E-26
2	2.98E-19	3.11E-21	3.15E-21	6.26E-21	1.40E-23
5	1.37E-17	9.13E-20	9.02E-20	1.82E-19	6.36E-21
10	1.14E-16	6.02E-19	5.78E-19	1.18E-18	2.12E-19
20	4.33E-16	2.60E-18	2.40E-18	5.00E-18	3.48E-18
50	8.65E-16	1.13E-17	9.84E-18	2.12E-17	5.55E-17
100	8.45E-16	2.68E-17	2.24E-17	4.93E-17	1.72E-16

Table 6. *Reaction Rate Data based on the equations developed by Bosch and Hale.*

It is important to note that Bosch and Hale give temperature ranges over which this approximation is valid. Table 7 shows the starting and ending temperatures over which the approximation is valid. This validity range is evident when the reactivities are plotted over a large range of values. Figure 1 shows the reaction rate plots for each of the fusion reactions from 1 keV to 10 MeV. Note that the reactivity approximation for $D(d,n)^3He$ has an asymptote at approximately 1 MeV.

Reaction	Minimum Temperature (keV)	Maximum Temperature (keV)
$T(d,n)^4He$	0.2	100.0
$D(d,n)^3He$	0.2	100.0
D(d,p)T	0.2	100.0
$^3He(D,p)^4He$	0.5	190.0

Table 7. *R-matrix temperature confidence intervals for each of the given fusion reactions.*

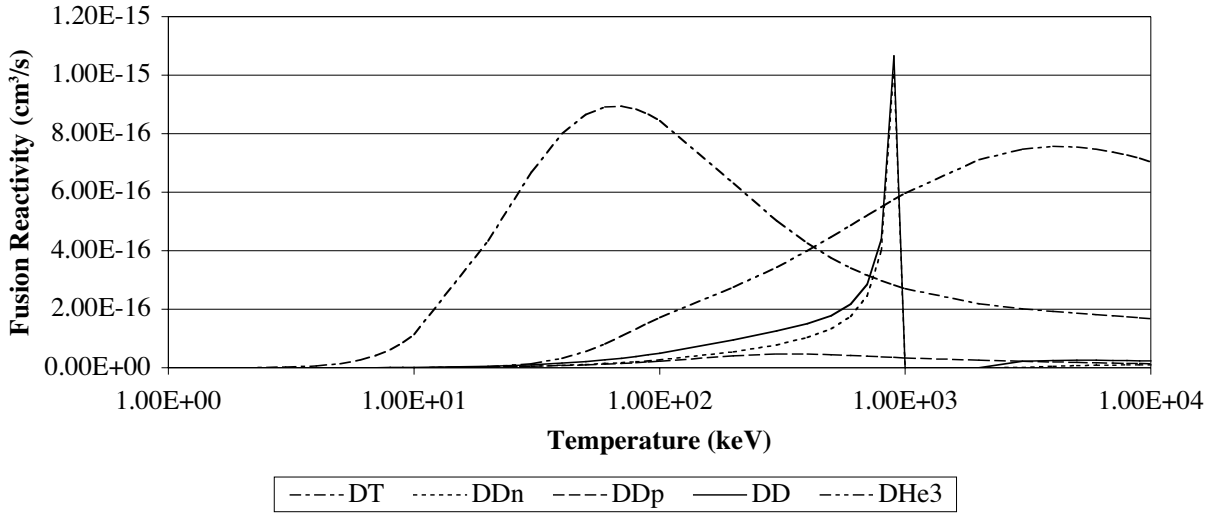

Figure 1. *The fusion reactivity plots for each of the fusion reaction species as a function of energy from 1 keV to 10 MeV.*

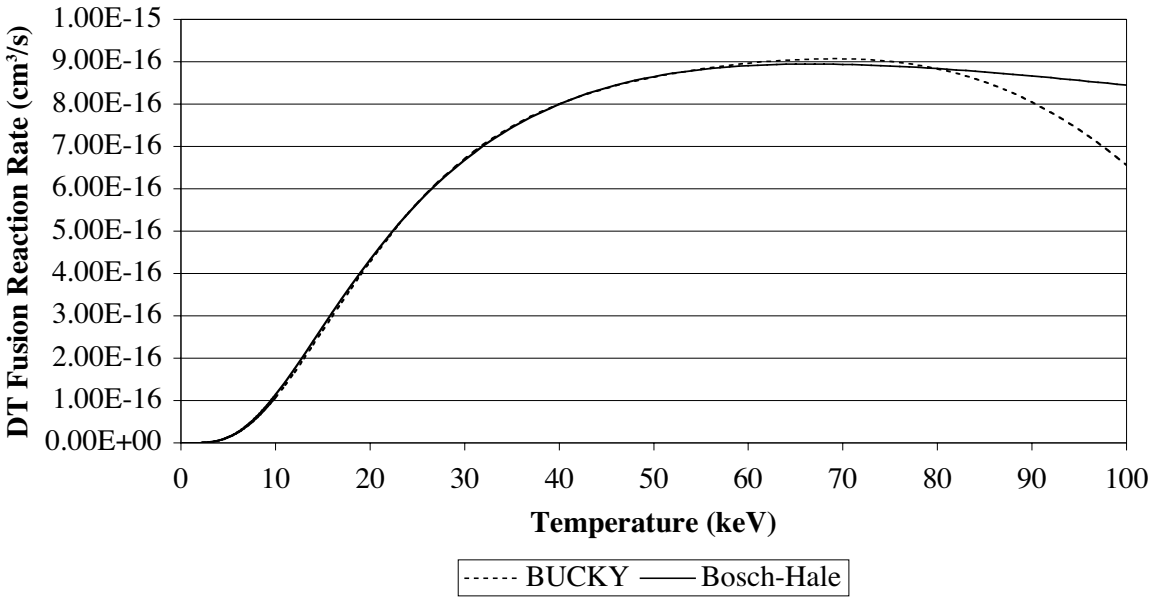

Figure 2*. A comparison of the BUCKY and Bosch-Hale reactivities for the T(d,n)^{4}He reaction from 0.1 keV to 100.0 keV.*

Reactivity Comparison

Now that the different formulations for fusion reactivities have been examined, we can compare the Bosch-Hale results to the data described earlier in this paper. Using the Bosch-Hale formulation as a baseline, the relative error of the values from the NRL Plasma Formulary, DRACO tabulated data and BUCKY fitting equations for the T(d,n)^{4}He fusion reaction is given in Table 8. There are two noteworthy features of this error analysis: that the relative error is largest at low temperatures, as was expected; also that the approximation used by BUCKY is not valid for temperatures higher than ~50 keV. Figure 2 shows a plot of the BUCKY approximation compared to the Bosch-Hale approximation, where the deviation of the BUCKY approximation at high energies is clearly evident.

Temperature (keV)	ε_{DT}, NRL (%)	ε_{DT}, DRACO (%)	ε_{DT}, BUCKY (%)
1	19.79	20.08	20.03
2	12.68	12.00	12.16
5	4.82	4.82	4.97
10	3.18	4.94	5.10
20	3.01	1.16	1.18
50	0.59	0.11	0.11
100	0.62	0.62	22.30

Table 8. *The relative error of the NRL, DRACO and BUCKY reactivities from the Bosch-Hale reactivity for the $T(d,n)^4He$ fusion reaction.*

Similarly, the relative error analysis for the sum of $D(d,n)^3He$ and D(d,p)T fusion reactions was performed. As with the data for the $T(d,n)^4He$ reaction, the DD_{total} reaction rates deviate the greatest at low temperatures. It is also evident from the error analysis in Table 9 that the formulation used in BUCKY overpredicts the fusion reactivity at all energies – even when compared to the older reactivity formulations found in the NRL Plasma Formulary and the tabulated data found in DRACO. This overprediction of reaction rates is clearly evident in the reactivity plot given in Figure 3.

Temperature (keV)	ε_{DD}, NRL (%)	ε_{DD}, DRACO (%)	ε_{DD}, BUCKY (%)
1	25.37	24.27	57.63
2	13.74	13.42	52.55
5	0.84	2.38	45.03
10	1.66	2.25	36.17
20	3.97	3.17	18.51
50	0.79	1.93	66.01
100	8.64	5.80	492.07

Table 9. *The relative error of the NRL, DRACO and BUCKY reactivities from the Bosch-Hale reactivity for the DD_{total} fusion reaction.*

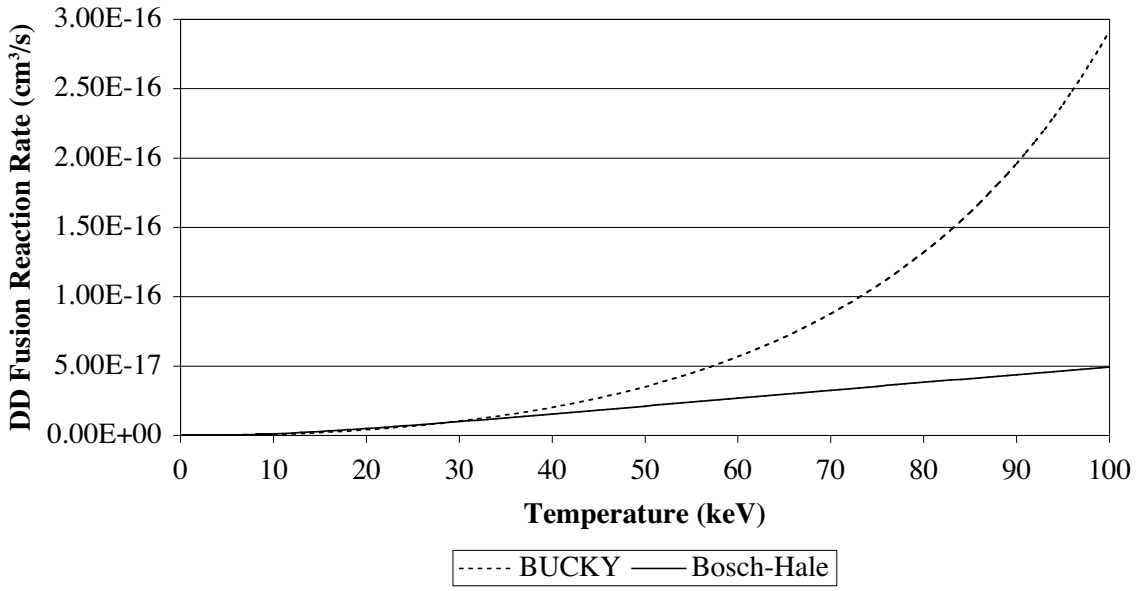

Figure 3. *A comparison of the BUCKY and Bosch-Hale reactivities for the DD_{total} reaction from 0.1 keV to 100.0 keV.*

Lastly, the $^3He(D,p)^4He$ reaction rate relative error was calculated. Unlike the previous two reaction models, the Bosch-Hale reaction rate model agrees fairly well with the DRACO tabulated data and BUCKY approximation over all of the given temperatures. As shown in Table 10, the greatest deviation from the Bosch-Hale results occurs in the 10-20 keV temperature range. The large deviation found in the NRL Plasma Formulary data is accounted for by the fact that that reactivity was given as an order of magnitude approximation, not an actual reaction rate value. Figure 4 shows the comparison of the DRACO approximation to the Bosch-Hale approximation.

Temperature (keV)	ε_{DHe3}, NRL (%)	ε_{DHe3}, DRACO (%)	ε_{DHe3}, BUCKY (%)
1	67.17	0.84	0.75
2	0.33	1.77	1.86
5	5.28	4.50	4.46
10	8.36	7.41	7.37
20	9.27	8.98	8.86
50	2.69	1.60	1.69
100	6.83	6.83	1.30

Table 10. *The relative error of the NRL, DRACO and BUCKY reactivities from the Bosch-Hale reactivity for the $^3He(D,p)^4He$ fusion reaction.*

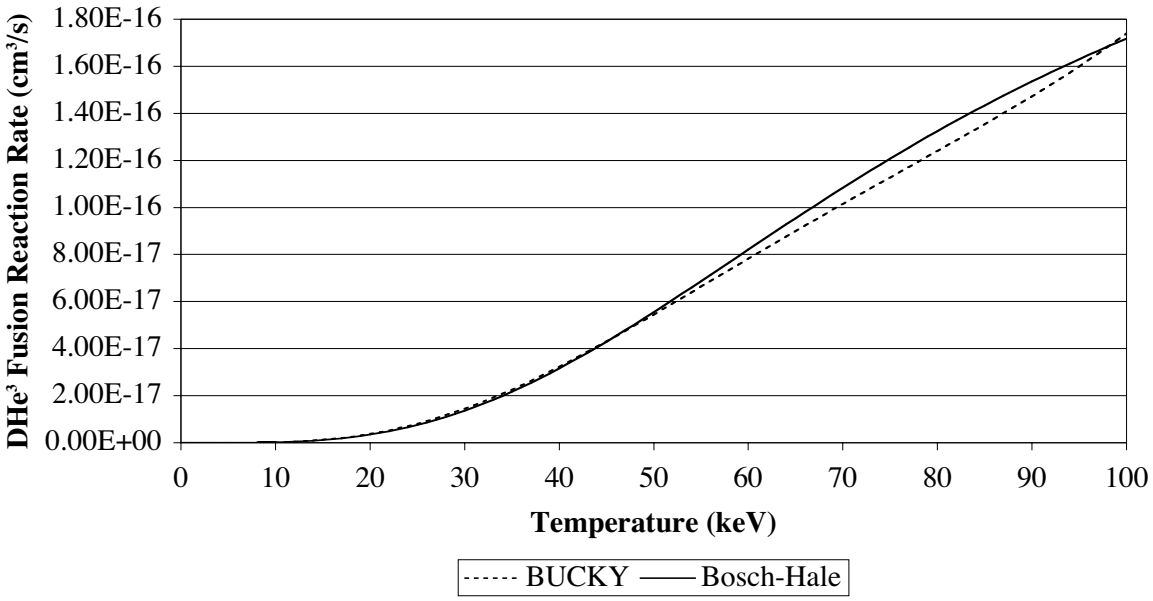

Figure 4. *A comparison of the BUCKY and Bosch-Hale reactivities for the $^3He(D,p)^4He$ reaction from 0.1 keV to 100.0 keV.*

Timing Study

A timing study of the BUCKY and Bosch-Hale reactivity equations was done to determine whether the Bosch-Hale reactivity model would be significantly more expensive to compute compared to the reactivity model used in BUCKY. A C++ program (Appendix II) was written to output reactivities based on an input temperature. A perl script was then written (Appendix III) to iterate through input temperatures for both reactivity equations. The programs were run on a Macintosh PowerBook with a 1 GHz G4 processor, 1 GHz of system RAM and running OS 10.3.7. The input energy was iterated from 0.2 keV to 100.0 keV in increments of 0.01 keV for a total of 9980 calls to the program for each reactivity model. The results of the timing study are given in Table 11.

Reactivity Model	Start Time (T = 0.2 keV)	End Time (T = 100.0 keV)	Difference (s)
BUCKY	1105128774.0±0.5	1105129184.0±0.5	410.0±1.0
Bosch-Hale	1105129184.0±0.5	1105129598.0±0.5	414.0±1.0

Table 11. *The timing data for 9980 calls to the test function containing both the BUCKY and Bosch-Hale reactivity equations.*

It was noted that the Bosch-Hale reactivity computations took 4.0±1.0 seconds (0.98±0.24%) longer to complete than the current BUCKY reactivity model. The timing results indicate that implementing the Bosch-Hale reactivity model would not be significantly more computationally expensive than the existing BUCKY reactivity model.

Conclusion

For a slight increase in computational expense (approx. 1%), implementing the Bosch-Hale R-matrix fusion reaction rate model would result in more accurate reaction rates at low plasma temperatures (<100 keV). It has been shown that for the fusion reaction rate modeled in BUCKY that implementing the R-matrix reaction rate model would increase the accuracy of the fusion reactivities over all desired plasma temperatures. The greatest improvement would be in the D(d,n)^{3}He and D(d,p)T reaction rates, which are being overpredicted in the current BUCKY model.

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Appendix I

The figures from [2] which are referenced in the paper have been reproduced below:

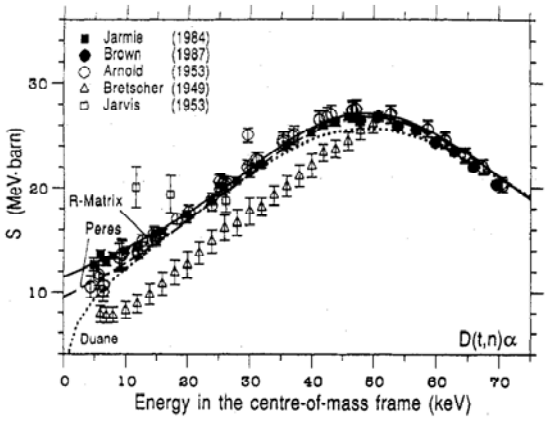

FIG. 2. S-values as a function of the energy available in the CM frame for the d + t reaction. The S-values were derived from the experimental data mentioned in the figure. Bretscher's data [44] are much too low and do not show the maximum, while Jarvis' data [34] do not even follow the trend of the data. The new Los Alamos data confirm quite well the measurements of Arnold et al. [33], except at the very low energies, where Arnold's data are too low.

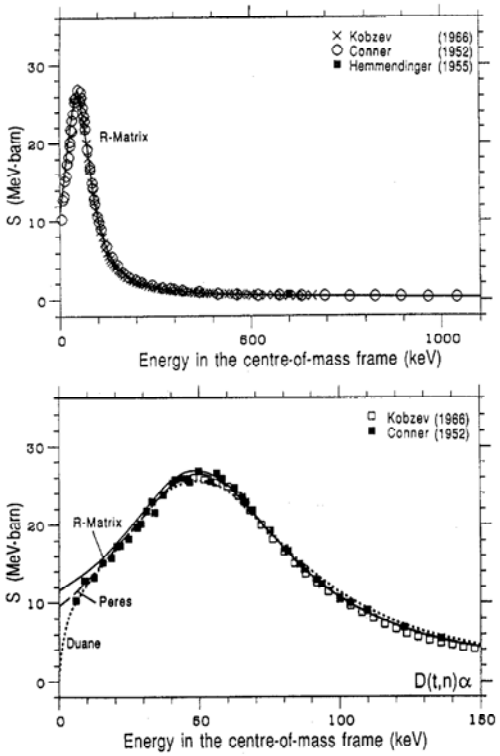

FIG. 3. S-values as derived from the measurements of Katsaurov [41] in 1962 (also published by Kobzev et al. [40] in 1966) and from Conner et al. [28] in 1952. The error bars given by these authors are smaller than the symbol size in this figure and they have therefore been omitted. Data have been published for energies up to 1 MeV, but this figure has been restricted in order to show the region of the resonance in greater detail. These data agree very well with the parametrizations of Duane and of Peres, and they are a little lower than the R-matrix evaluation.

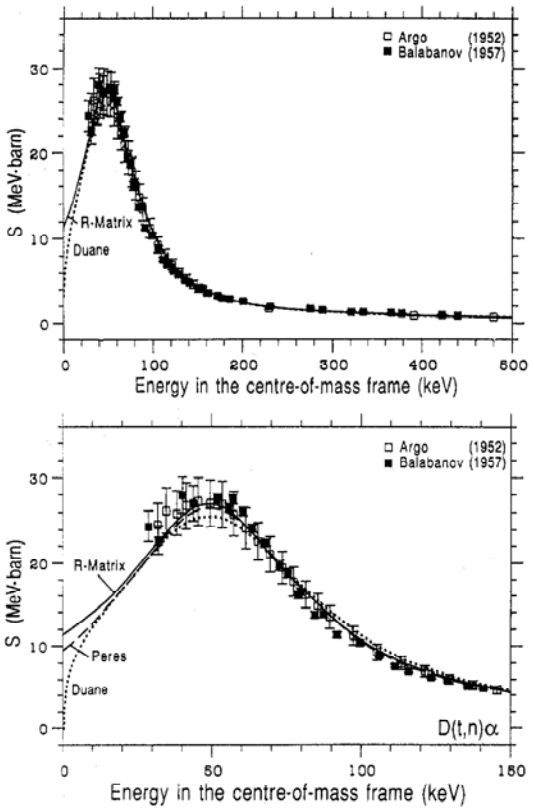

FIG. 4. S-values as derived from the measurements of Argo et al. [27] in 1952 and from Balabanov et al. [38] in 1957. The error bars are quite large in the region of the resonance, but the data are even above the values from the R-matrix calculation. Again, this figure shows only a part of the data which have been measured up to 500 keV.

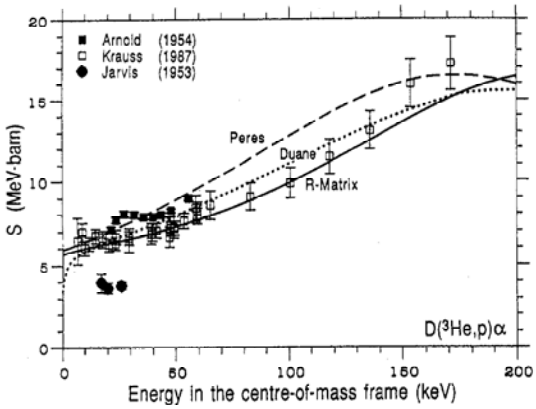

FIG. 5. S-values as a function of the energy available in the CM frame for the d + ^{3}He reaction. Jarvis' data [34] are much too low and should not be used for any evaluation. Krauss' data [50] were measured long after the R-matrix had been calculated, but they agree rather well with it, except for the two points at the highest energies.

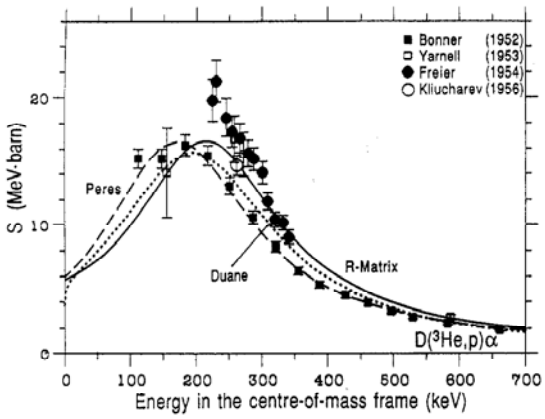

FIG. 6. S-values as a function of the energy available in the CM frame for the d + ^{3}He reaction. It was mainly the dataset of Bonner [45] that determined Peres' fit, as can be seen here.

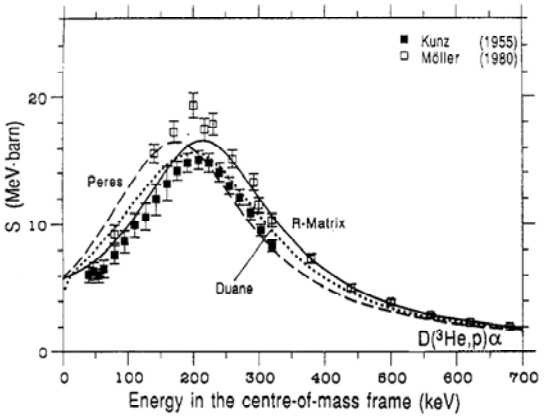

FIG. 7. S-values as a function of the energy available in the CM frame for the d + ^{3}He reaction. The data of Möller et al. [49] were taken after the R-matrix calculation, but they agree rather well with these results, except in the region just below the resonance.

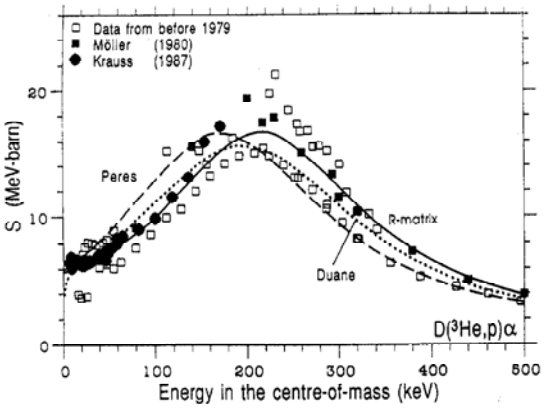

FIG. 8. S-values as a function of the energy available in the CM frame for the d + ^{3}He reaction. The light squares mark all the data taken before 1960, and the solid line shows the results of the R-matrix calculation from 1979, based on these data and on data for other reactions. The dark symbols show the data taken later, which agree rather well with these R-matrix results, except for some discrepancy in the region of the resonance.

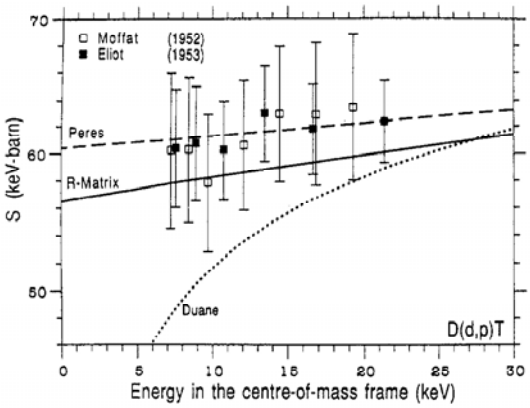

FIG. 9. S-values as a function of the energy available in the CM frame for the D(d,p)T reaction. Although both datasets have appreciable error bars assigned to them, they clearly disagree with the trend of Duane's parametrization.

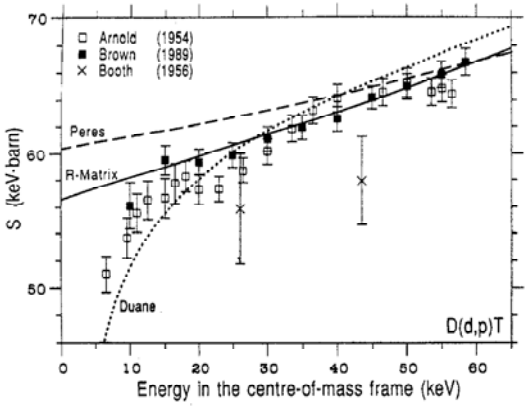

FIG. 10. S-function of the D(d,p)T reaction. Arnold's data [30] (points of a smooth curve through the experimental data) decrease sharply towards low energies, unlike all other datasets. The data of Booth et al. [62] are much lower than all the other data and should not be used for a parametrization.

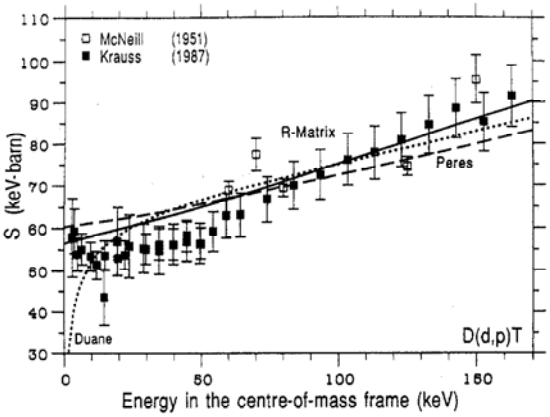

FIG. 11. S-function of the D(d,p)T reaction. Krauss et al. [50] used two different accelerators for their measurements, and the very low data point at about 15 keV is the lowest energy point of the high energy accelerator experiments.

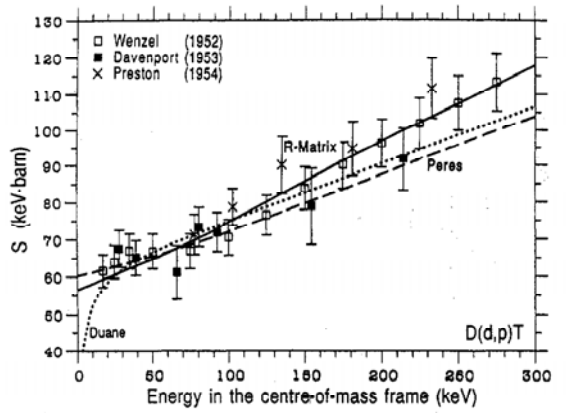

FIG. 12. S-function of the D(d,p)T reaction. The data of Wenzel and Whaling [61] and those of Preston et al. [59] are much higher than the old parametrizations for energies above about 200 keV.

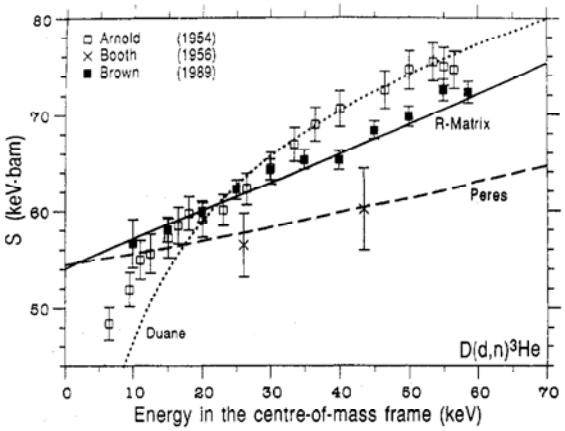

FIG. 13. S-function of the D(d,n)^{3}He reaction. As in the case of the D(d,p)T reaction, Arnold's data [30] decrease sharply towards low energies, unlike all other datasets, and again the data of Booth et al. [62] are too low. Arnold's data have been corrected as described in the text.

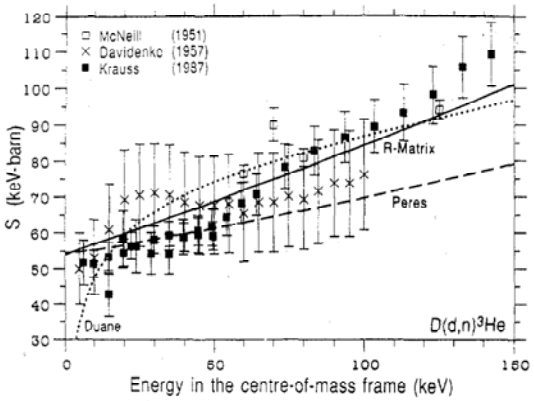

FIG. 14. S-function of the D(d,n)^{3}He reaction. The data of McNeill and Keyser [60] have been corrected as described in the text.

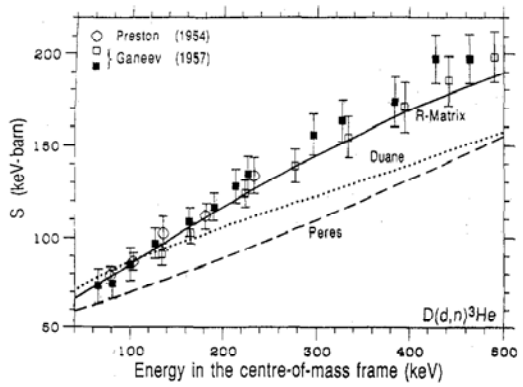

FIG. 15. S-function of the D(d,n)^{3}He reaction for higher energies. Ganeev et al. [69] used two different methods — numerical integration of differential cross-sections (light squares) and measurements in a $KMnO_4$ bath (black squares). Again, in this energy region all experimental data are higher than the old parametrizations and agree with the R-matrix results.

Appendix II

The source code used to analyze the timing information for the BUCKY and Bosch-Hale <σv> calculations is given below:

```
#include <iostream>
#include <math.h>
#include <stdlib.h>

int main (int argc, char * const argv[]) {
        // This function returns the < sigma*v > value based on the paper
        // "Improvised Formulas for Fusion Cross-Sections and Thermal Reactivities"
        // H.S. Bosch, G.M. Hale
        // Nuclear Fusion, Vol. 32, No. 4 (1992) Pp. 611-631
        //
        // The < sigma*v > values are valid for ion temperatures:
        // 0.2-100 keV for T(d,n)4He
        // 0.5-190 keV for 3He(d,p)4He
        // 0.2-100 keV for D(d,p)T
        // 0.2-100 keV for D(d,n)3He
        //
        // Input Parameter(s): T_ion [keV], < sigma*v > model desired [1=BUCKY, 2=Bosch-Hale]
        // Output(s): < sigma*v > for each of the reactions given above [cm^3/s]
        //
        // Created: 20 Dec, 2004
        //          Thad  A. Heltemes

        //std::cout << "Received " << argc << " arguments...\n";
        //for (int i=0; i<argc; i++)
        //      std::cout << "Argument " << i << ": " << argv[i] << "\n";

        char * pEnd;
        double Tion = strtod(argv[1], &pEnd);
        int model = atoi(argv[2]);
        double sigmav[4];

        printf("T_ion = %f keV\n\n", Tion);

        if (model == 1) {
                double r[3]  = {         0.2935,         0.3735,         0.3597 };
                double A1[3] = { -2.1377692E+01, -1.5511891E+01, -2.7764468E+01 };
                double A2[3] = { -2.5204050E+01, -3.5318711E+01, -3.1023898E+01 };
                double A3[3] = { -7.1013427E-02,  1.2904737E-02,  2.7889999E-02 };
                double A4[3] = {  1.9375450E-04,  2.6797766E-04, -5.5321633E-04 };
                double A5[3] = {  4.9246592E-06, -2.9198658E-06,  3.0293927E-06 };
                double A6[3] = { -3.9836572E-08,  1.2748415E-08, -2.5233325E-09 };

                for (int i=0; i<3; i++) {
                        sigmav[i] =
exp((A1[i]/(pow(Tion,r[i])))+A2[i]+A3[i]*Tion+A4[i]*pow(Tion,2)+A5[i]*pow(Tion,3)+A6[i]*pow(Tion,
4));
                        printf("BUCKY Reaction %d, < s*v > = %e\n", i, sigmav[i]);
                }
                printf("Reactions: 0=DT, 1=DD, 2=DHe3\n");
        }

        else if (model == 2) {
                double Theta;
                double X;

                double mrc2[4] = { 1.124656E+06, 1.124572E+06, 9.37814E+05,  9.37814E+05 };
                double BG[4]   = {      34.3827,      68.7508,     31.3970,      31.3970 };
                double C1[4]   = {  1.17302E-09,  5.51036E-10, 5.65718E-12,  5.43360E-12 };
                double C2[4]   = {  1.51361E-02,  6.41918E-03, 3.41267E-03,  5.85778E-03 };
                double C3[4]   = {  7.51886E-02, -2.02896E-03, 1.99167E-03,  7.68222E-03 };
                double C4[4]   = {  4.60643E-03, -1.91080E-05, 0.00000E+00,  0.00000E+00 };
                double C5[4]   = {  1.35000E-02,  1.35776E-04, 1.05060E-05, -2.96400E-06 };
                double C6[4]   = { -1.06750E-04,  0.00000E+00, 0.00000E+00,  0.00000E+00 };
```

```
                double C7[4]   = {  1.36600E-05,  0.00000E+00, 0.00000E+00,  0.00000E+00 };

                if (Tion < 0.2 || Tion > 100.0) { printf("WARNING: Outside of Confidence Interval
(0.2-100.0 keV)\n"); }
                for (int i=0; i<4; i++) {
                        Theta = Tion/(1-
((Tion*(C2[i]+Tion*(C4[i]+Tion*C6[i])))/(1+Tion*(C3[i]+Tion*(C5[i]+Tion*C7[i])))));
                        X = pow(((BG[i]*BG[i])/(4.*Theta)),(1./3.));
                        sigmav[i] = C1[i]*Theta*sqrt(X/(mrc2[i]*pow(Tion,3.)))*exp(-3.*X);
                        printf("Bosch-Hale Reaction %d, < s*v > = %e\n", i, sigmav[i]);
                }
                printf("Reactions: 0=DT, 1=DHe3, 2=DD->p, 3=DD->n\n");
        }

        else {
                printf("FATAL Error! Not a valid option!\n");
        }
        return 0;
}
```

Appendix III

The perl script used to iterate through the ion temperatures for the BUCKY and Bosch-Hale timing information is given below:

```
#!/usr/bin/perl
#
# This script is used to get timing information for multiple
# iterations of an executable.
#
# 12/30/04 - TAH
#

$start = 0.20;
$end = 100.00;
$increment = 0.01;

printf("Timing start at %f = %d\n", $start, time);
while ($start <= $end) {
        system "./test $start $ARGV[1] > /dev/null";
        $start += $increment;
}
printf("Timing end at %f = %d\n", $end, time);
```