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## Reactivities of neutronic and aneutronic fusion fuels

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#### 1. Introduction

Nuclear fusion research relies on two types of fuels, viz., neutronic and aneutronic. In case of neutronic fuels, one of the byproducts is neutron (Atzeni and Meyer-ter vehn, 2004; Dawson, 1981). Most widely considered neutronic fuels are DT, DD, TT and THe<sup>3</sup>. Among these fuels, DT, DD and TT are considered as first generation fuels since these are isotopes of hydrogen. Aneutronic fusion fuels have the advantage that they reduce neutron induced radioactivity. Often considered aneutronic fuels are DHe<sup>3</sup>, Li<sup>6</sup>He<sup>3</sup>, Dp and He<sup>3</sup>He<sup>3</sup>. Many authors have considered DHe<sup>3</sup> as the cleanest fuel (Son and Fisch, 2004; Rand McNally, 1971), however, the occurrence of side reactions (DD and DT) is unavoidable. Technical difficulties arising in the use of pure DT can be reduced by using DHe<sup>3</sup> fuel (Honda et al., 1991). Also, DHe<sup>3</sup> fuel is used in satellite reactors (Miley et al., 1977). Apart from this, the probability of interaction is significant when ion temperature exceeds 50 keV (Son and Fisch, 2004). Fusion reactions with lithium (or its isotopes) like Li<sup>6</sup>He<sup>3</sup> are of current interest due to abundant availability of Li in nature. Also, Dp and He<sup>3</sup>He<sup>3</sup> fusion reactions are important since they occur in the p-p cycle of Sun (Clayton, 1968).

Reaction probability between two interacting nuclei is characterized by fusion cross-section. The Maxwellian average of the product of cross-section and relative velocity of the two interacting nuclei defines fusion reactivity. In other words, reaction rate is the probability of interactions per unit time per unit number density of target nuclei (Atzeni and Meyer-ter vehn, 2004; Duderstadt and Moses, 1982). Possibility of efficient thermonuclear burn in a

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#### ABSTRACT

Fusion reactivities ( $\langle \sigma v \rangle$ ) of some neutronic and aneutronic fusion fuels are evaluated numerically using cross-section data available from IAEA site. Comparison of new reactivities with the fitting formula published in earlier works shows that these fits are accurate only in certain temperature ranges. Here, new polynomial fits for fusion reactivities are proposed. Agreement of the new fittings with numerical values of  $\langle \sigma v \rangle$  is found to be quite good.

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fusion system strongly depends on fusion reactivity (Avrorin et al., 1980; Kawata et al., 1982; Takase et al., 1983; Basko, 1990; Kawata and Nakashima, 1992; Frolov et al., 2002; Nayak and Menon, 2012). For self-sustained burning, fusion energy production should exceed radiation losses (bremsstrahlung, synchrotron, black-body).

Temperature dependence of  $\langle \sigma v \rangle$  gives idea of the temperature regime in which burn-up is feasible. Several fitting formulas of reaction rate of neutronic fuels available in literature are valid in low temperature regimes (Huba, 2009; Tuck, 1961; Frolov, 1998; Hively, 1977, 1983; Brueckner and Jorna, 1974). Numerical and graphical data of  $\langle \sigma v \rangle$  for DT, DD and DHe<sup>3</sup> are published (Huba, 2009; Tuck, 1961; Bosch and Hale, 1992). Futch has determined reaction rate of DT and DHe<sup>3</sup> by solving Fokker–Planck equations in thermal plasma (Futch et al., 1972).

Our aim is this paper is to study  $\langle \sigma v \rangle$  as a function of temperature for all the fuels described above. We also propose new polynomial fittings of  $\langle \sigma v \rangle$  in a wide temperature range 0.1 keV to 10 MeV. These fittings are useful in burn-up calculations. The paper is organized as follows. Section 2 contains fusion reactions of all fuels mentioned above and the expression for fusion reactivity. Section 3 summarizes most of the existing fittings of reaction rate. In Section 4, numerical comparison of fusion reactivity and polynomial fittings are given. We conclude the paper in Section 5.

#### 2. Fusion reactions and reaction rate

#### 2.1. Neutronic fuels

Neutronic fuels are those in which one of the byproducts is neutron. Neutronic fuels considered in this paper are given below:





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$$_{1}D^{2} + _{1}T^{3} \rightarrow _{2}He^{4} + _{0}n^{1} + 17.6 \text{ MeV}$$
 (1)

$${}_{1}D^{2} + {}_{1}D^{2} \rightarrow {}_{2}He^{3} + {}_{0}n^{1} + 3.27 \text{ MeV}$$

$${}_{1}D^{2} + {}_{1}D^{2} \rightarrow {}_{1}T^{3} + {}_{1}p^{1} + 4.03 \text{ MeV}$$

$$(2)$$

$$_{1}T^{3} + _{1}T^{3} \rightarrow _{2}He^{4} + 2_{0}n^{1} + 11.33 \text{ MeV}$$
 (3)

$$_{1}T^{3} + _{2}He^{3} \rightarrow _{2}He^{4} + _{0}n^{1} + _{1}p^{1} + 12.1 \text{ MeV}$$
 (4)

Among all the four reactions, energy released in DT fusion is highest. Also,  $_1T^3$  produced in DD-p channel reacts with  $_1D^2$ . Fusion cross-section of THe<sup>3</sup> is relatively smaller due to the high barrier potential.

#### 2.2. Aneutronic fuels

Fusion reactions of aneutronic fuels considered below are the following:

$$_{1}D^{2} + _{2}He^{3} \rightarrow _{2}He^{4} + _{1}p^{1} + 18.35 \text{ MeV}$$
 (5)

 $_{3}\text{Li}^{6} + _{2}\text{He}^{3} \rightarrow 2_{2}\text{He}^{4} + _{1}p^{1} + 16.9 \text{ MeV}$  (6)

 $_{1}D^{2} + _{1}p^{1} \rightarrow _{2}He^{3} + \gamma + 5.49 \text{ MeV}$  (7)

$$_{2}\text{He}^{3} + _{2}\text{He}^{3} \rightarrow _{2}\text{He}^{4} + 2_{1}\text{p}^{1} + 12.86 \text{ MeV}$$
 (8)

Fusion energy released in DHe<sup>3</sup> reaction is maximum. Dp and  $He^{3}He^{3}$  fusion reactions take place in p-p cycle.

Fusion reactivity is defined as the Maxwellian average of the product of the fusion cross-section and the relative velocity of reacting nuclei. Thus  $\sigma v$  is averaged over the whole range of velocities of two nuclei, as they follow Maxwellian distribution of velocities (or energies) (Atzeni and Meyer-ter vehn, 2004; Duderstadt and Moses, 1982). The expression of  $\langle \sigma v \rangle$  is given by:

$$\langle \sigma \nu \rangle = \left(\frac{m_r}{2\pi k_B T}\right)^{3/2} \int_{-\infty}^{\infty} \sigma(\nu) \ \nu \ exp\left(-\frac{m_r \nu^2}{2k_B T}\right) d^3\nu \tag{9}$$

where  $\sigma(v)$ , v and  $m_r$  are, respectively, the fusion cross-section, relative velocity of two colliding nuclei and their reduced mass. In a fusion reaction, ions either overcome the potential barrier or penetrate through it. Probability of these two phenomena determines the fusion cross-section. The functional form of  $\sigma(v)$  is given by Duderstadt and Moses (1982):

$$\sigma(\nu) = \frac{A_1}{\nu^2} \exp\left(-\frac{B_1}{\nu}\right) \tag{10}$$

where  $A_1$  and  $B_1$  are constants characterizing a particular reaction. In terms of laboratory energy *E* the reactivity can be written as:

$$\langle \sigma \nu \rangle = \frac{4}{\sqrt{2\pi}} \left(\frac{m_r}{k_B T}\right)^{3/2} \frac{1}{m_1^2} \int_0^\infty \sigma(E) \ E \ \exp\left(-\frac{m_r}{m_1} \frac{E}{k_B T}\right) dE \tag{11}$$

#### 3. Existing fits for reaction rates

Fittings of reaction rate have been carried out by many authors. The fits for DT and DD reactions given in Brueckner–Jorna (1974) involves two different temperature regimes, i.e. T > 10 keV and T < 10 keV (Brueckner and Jorna, 1974). Hively (1977) has proposed parametric fits of  $\langle \sigma v \rangle$  in the range 1 keV  $\leq T \leq 80$  keV for DT, DD and DHe<sup>3</sup> by using a least square method (Hively, 1977). He proposed new fittings for DT and DHe<sup>3</sup> later (1984). These formula for DT is 10% accurate in the temperature range 3–100 keV and 20% accurate in the range 0.3–3 keV, whereas for DHe<sup>3</sup>, they are accurate to 10% in the range 0.5–100 keV.

In 1992 thermal reactivities have been calculated numerically on the basis of new R-matrix cross-section by Bosch and Hale (1992). For DT and DD fusion, the fittings are accurate in the regime 0.2–100 keV but for DHe<sup>3</sup> it is accurate in 0.5–190 keV. Recently in 2009, fittings of reaction rate of all the neutronic fuels are tabulated in NRL formulary in the temperature limit 1 keV  $\leq T \leq$  1000 keV (Huba, 2009).

#### 4. New evaluation of reactivity and fits

#### 4.1. Numerically calculated reactivity

To evaluate  $\langle \sigma v \rangle$ , we have used point cross-section data,  $\sigma(E)$  vs. *E* from IAEA site. These point values are then interpolated by quadratic polynomial functions in two small neighboring energy segments in the tabulations. Proper care is taken in the starting and final segments. Then, for a particular temperature, the integration in Eq. (11) is performed for those segments using adaptive Simpson rule (Press et al., 1993). Thus with the use of piecewise interpolation and subsequent integration scheme we have evaluated fusion reactivity for the entire energy range. This method is repeated for all temperatures in the range 0.1 keV to 10 MeV.

#### 4.2. Polynomial fits of reaction rate

Thermonuclear burn-up calculations require accurate data of reaction rates. Use of numerical integration of reactivity for burn-up calculations increases calculation time to unacceptable levels. Therefore, accurate fitting formulas of fusion reactivity are very useful. Here, new polynomial fittings are proposed for all the different fuels applicable in a wide temperature range: 0.1 keV to 10 MeV. The order of polynomial function is decided by determining the minimum value of deviation or error,  $\Delta$ , defined as the sum of square of relative differences between numerical and fitted values for all temperature in the range 0.1 keV to 10 MeV (http://hsl.rl.ac.uk/archive/cou.html). The expression used for the best polynomial order is given below:

$$\langle \sigma \nu \rangle = 10^{a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + a_6 x^6 + a_7 x^7} \tag{12}$$

where  $x = log_{10}T$ . The set of constants  $(a_i)$  are reaction specific. The total relative errors,  $\triangle$ , were determined for different orders of the polynomial. These are given in Tables 1 and 2 for neutronic and aneutronic fusion reactions, respectively. We find from Table 1 that the total relative errors  $(\triangle)$  for DD reaction decrease rapidly with increase in polynomial order. Even if for 7th order polynomial,  $\triangle$  value is one order magnitude less than for other three and it continues up to 9th order. From 3rd to 10th order, the total error estimated for TT and THe<sup>3</sup> are very close. In case of DT, error reduces slowly as we see from second column. All reactions have similar  $\triangle$  for 10th order polynomial fit.

In all neutron less fuels, Dp has large relative errors. For 3rd order fit,  $\triangle$  for Dp is 36.427, while it reduces to 0.105 at 7th order. For all cases  $\triangle$  decreases with increase in polynomial order except for Li<sup>6</sup>He<sup>3</sup>. For this fuel, error corresponding to 7th order polynomial (0.008) is less than 9th (0.011) and 10th (0.009) order fits. Higher

Table 1		
Polynomial order vs.	total relative error ( $\varDelta$ ) of neutronic fusion reactions.	

Polynomial order	DT	DD	TT	THe <sup>3</sup>
3	0.917	0.235	0.380	0.259
4	0.223	0.009	0.015	0.017
5	0.012	0.003	0.006	0.016
6	0.006	0.001	0.002	0.009
7	0.002	0.0004	0.002	0.002
8	0.002	0.0004	0.001	0.001
9	0.001	0.0002	0.001	0.001
10	0.0002	0.0002	0.0002	0.0002

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