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PREDICTED METHODS OF CHANGING THE MUON CATALIZED FUSION CYCLING RATE

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ABSTRACT

The following paper uses an easily modifiable computerized simulation procedure to predict reaction yields of muo-fusion. Reaction yields are predicted under varying conditions without the explicit solution of rate equations. Condititions and methods of optimizing reaction conditions by controlling the concentrations of hydrogen isotopes are discussed. The effects of non-equilibrated manipulation of reaction components and intermediates are predicted.

I. INTRODUCTION

There are three steps to solving muo-fusion rate equations: the determination of the Gibb's free energy, the solution of equilibrium equations, and the solution of differential kinetic equations. An easily modifiable method of predicting reaction yields under varying conditions without the explicit solution of rate equations will be presented. The method enables the effects of non-equilibrated reaction components and intermediates to be quickly and accurately predicted.

The number of fusions observed during muon-catalyzed fusion is dependant upon many factors. Among the most important of these is the concentration of the various isotopes. For temperatures $\leq$ 500 K optimum yields during muon catalyzed D-T fusion are obtained when the concentration of DT is small in comparison to the concentration of D_2 and T_2. Recent analyses indicate that at high temperatures the cycling rate increases as the concentration of DT increases. Recent predictions also indicate that the presence of free T atoms in a reaction chamber will increase the cycling rate. Methods and effects of manipulating these reaction concentrations are disscussed.

II. DERIVATION OF EQUATIONS

In order to derive muon-catalyzed fusion kinetic equations we make several simplifing assumptions. There is experimental evidence to support some, but not all of these assumptions.

Assumptions:

1) All reactions are either first order or pseudo-first order (they may be accurately considered first order in kinetic equations).

This assumption has been shown to be accurate in all cases in which it has been tested, and is in agreement with current theory on muon reaction mechanics in the rest of the cases.[1] There is no proof that this assumption will hold for all conditions.

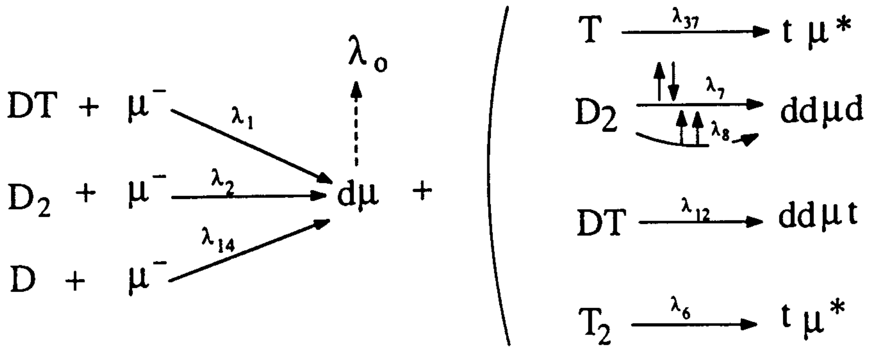
2) The transfer reaction $t\mu \longrightarrow d\mu$ may be considered negligible.

3) The $tt\mu$ muo–molecules do not form via resonance.

4) There are no significant reactions taking place other than those represented in the following diagrams. (Epithermal and hyperfine effects have not been included.)

Reaction Diagrams and Equations

The following diagrams and equations represent reactions which are predicted to occur during muon-catalyzed-fusion:[2] parallel arrows (↑↑) represent the reaction path of molecules with parallel nuclear spin, anti-parallel arrows (↑↓) represent the reaction path of molecules with anti-parallel nuclear spin, and Lambda (λ) represent rate constants. Not included in the diagrams or equations is the effect of muon scavenging by impurities in reaction chambers.



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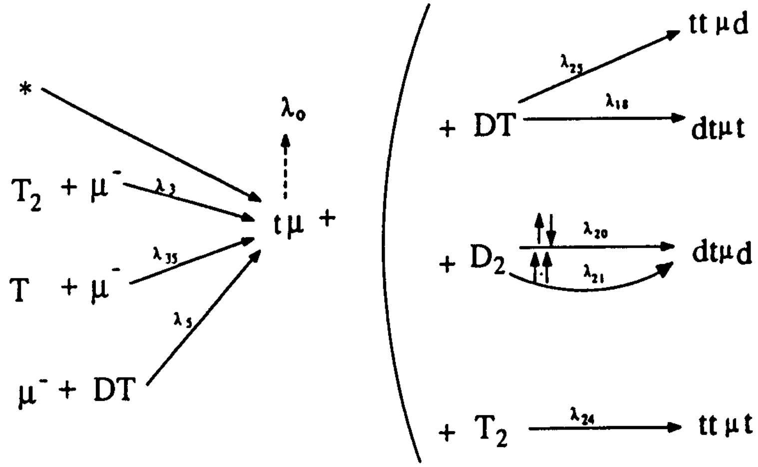
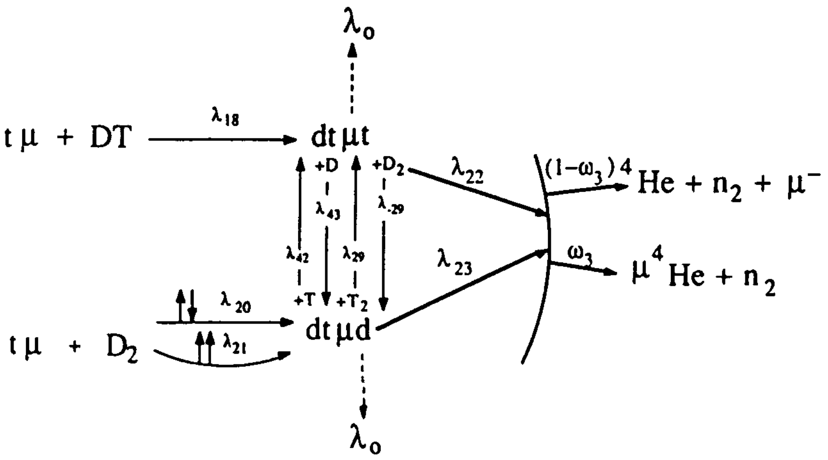
[1] Gershtein, **Sov. Phys. JETP**, 51(6), pp. 1053–1058.

[2] Jones, **Nature**,Vol 321, pp. 127–133.

$$\frac{d[d\mu]}{dt} = \lambda_1[DT][\mu^-] + [D_2][\mu^-] + \lambda_{14}[D][\mu^-] - \lambda_0[d\mu] - \lambda_{37}[d\mu][T] - (\lambda_7 + \lambda_8)[d\mu][D_2]$$
$$-\lambda_{12}[d\mu][DT] - \lambda_6[d\mu][T_2]$$

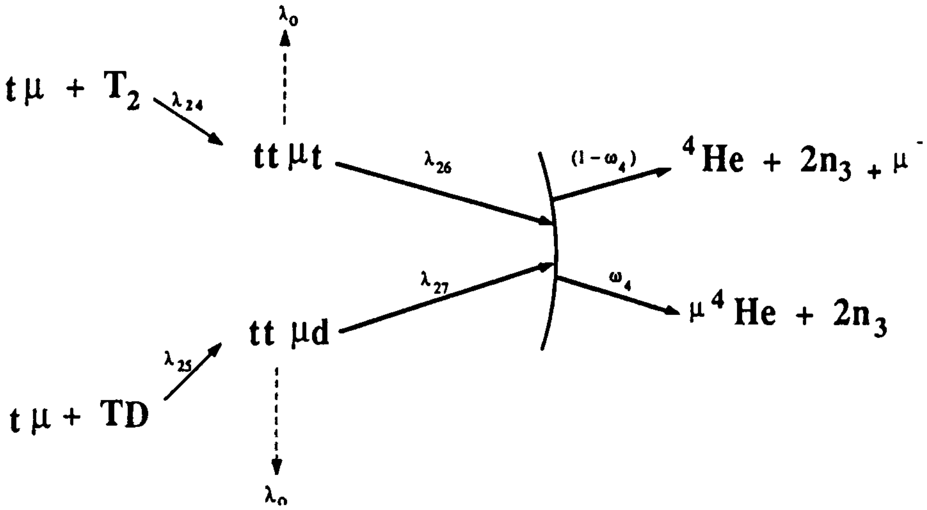


$$\frac{d[t\mu]}{dt} = \lambda_6[d\mu][T_2] + \lambda_{37}[d\mu][T] + \lambda_3[\mu^-][T_2] + \lambda_{35}[\mu^-][T] + \lambda_5[\mu^-][DT] - (\lambda_{25} + \lambda_{18})[t\mu][DT]$$
$$-(\lambda_{20} + \lambda_{21})[t\mu][D_2] - \lambda_{24}[t\mu][T_2]$$



$$\frac{d[dt\mu t]}{dt} = \lambda_{18}[t\mu][DT] + \lambda_{42}[T][dt\mu d] + \lambda_{29}[T_2][dt\mu d] - \lambda_{43}[D][dt\mu t]$$
$$-\lambda_{-29}[D_2][dt\mu t] - (\lambda_0 + \lambda_{22})[dt\mu t]$$

$$\frac{d[dt\mu d]}{dt} = (\lambda_{20} + \lambda_{21})[D_2][t\mu] + \lambda_{43}[D][dt\mu t] + \lambda_{-29}[D_2][dt\mu t] - (\lambda_0 + \lambda_{23})[dt\mu d]$$
$$-\lambda_{42}[T][dt\mu d] - \lambda_{29}[T_2][dt\mu d]$$



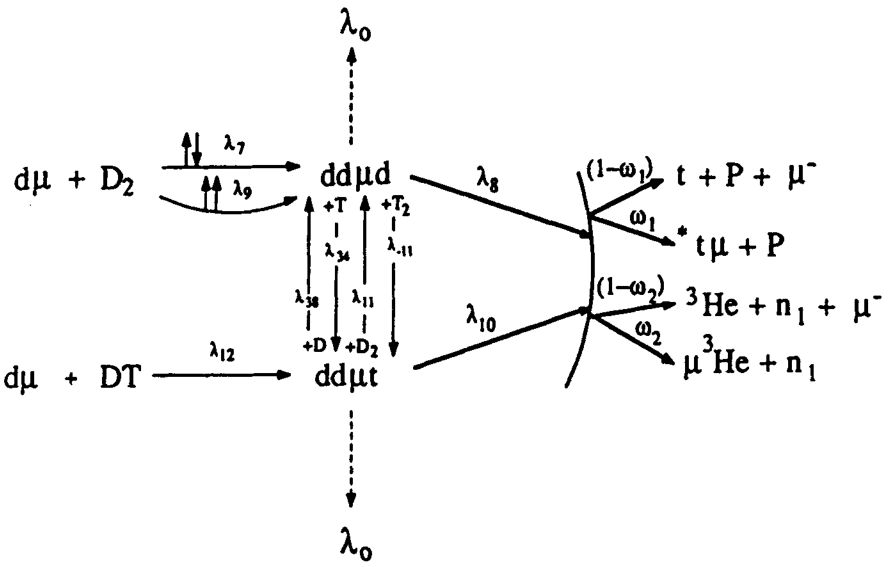
$$\frac{d[tt\mu t]}{dt} = \lambda_{24}[T_2][t\mu] - (\lambda_0 + \lambda_{26})[tt\mu t]$$

$$\frac{d[tt\mu d]}{dt} = \lambda_{25}[DT][t\mu] - (\lambda_0 + \lambda_{27})[tt\mu d]$$

$$\frac{d[dd\mu d]}{dt} = (\lambda_7 + \lambda_9)[D_2][d\mu] + \lambda_{38}[D][dd\mu t] + \lambda_{11}[D_2][dd\mu t] - (\lambda_0 + \lambda_8)[dd\mu d]$$
$$-\lambda_{34}[T][dd\mu d] - \lambda_{-11}[T_2][dd\mu d]$$

$$\frac{d[dd\mu t]}{dt} = \lambda_{12}[DT][d\mu] + \lambda_{34}[T][dd\mu d] + \lambda_{-11}[T_2][dd\mu d] - (\lambda_0 + \lambda_{10})[dd\mu t] -$$
$$\lambda_{38}[D][dd\mu t] - \lambda_{11}[D_2][dd\mu t]$$

$$\frac{d[\mu^-]}{dt} = \frac{1}{2}\{\lambda_8[dd\mu d] + \lambda_{10}[dd\mu t]\}(2 - \omega_1 - \omega_2) + \{\lambda_{22}[dt\mu t] + \lambda_{23}[dt\mu d]\}(1 - \omega_3)$$
$$+\{\lambda_{26}[tt\mu t] + \lambda_{27}[tt\mu d]\}(1 - \omega_4) - [\mu^-]\{\lambda_0 + \lambda_1[DT] + \lambda_2[D_2] + \lambda_{14}[D]$$
$$+\lambda_3[T_2] + \lambda_{35}[T] + \lambda_5[DT]\}$$



$$\frac{d[^3He]}{dt} = \frac{1}{2}\{\lambda_8[dd\mu d] + \lambda_{10}[dd\mu t]\}(1-\omega_2)$$

$$\frac{d[^3_\mu He]}{dt} = \frac{1}{2}\{\lambda_8[dd\mu d] + \lambda_{10}[dd\mu t]\}\omega_2$$

$$\frac{d[^4He]}{dt} = \{\lambda_{22}[dt\mu t] + \lambda_{23}[dt\mu d]\}(1-\omega_3) + \{\lambda_{26}[tt\mu t] + \lambda_{27}[tt\mu d]\}(1-\omega_4)$$

$$\frac{d[\mu^4He]}{dt} = \{\lambda_{22}[dt\mu t] + \lambda_{23}[dt\mu d]\}\omega_3 + \{\lambda_{26}[tt\mu t] + \lambda_{27}[tt\mu d]\}\omega_4$$

$$\frac{d[n_1]}{dt} = \frac{1}{2}(\lambda_8[dd\mu d] + \lambda_{10}[dd\mu t])$$

$$\frac{d[n_2]}{dt} = \lambda_{22}[dt\mu t] + \lambda_{23}[dt\mu d]$$

$$\frac{d[n_3]}{dt} = 2(\lambda_{26}[tt\mu t] + \lambda_{27}[tt\mu d])$$

$$\frac{d[n]}{dt} = \frac{d[n_1]}{dt} + \frac{d[n_2]}{dt} + \frac{d[n_3]}{dt}$$

III. DETERMINATION OF EQUILIBRIUM CONSTANTS

In order to determine the relative amounts of various hydrogen molecules which will be present in a reaction chamber at a given temperature and pressure, it is necessary to know the equilibrium constants (K_{eq}) of the gases involved. Equilibrium constants are most often calculated from the Gibb's free energy (ΔG) by the equation:[3]

$$\Delta G = -RT \ln K_{eq}$$

R = 8.3144
T is the temperature in degrees Kelvin

Values of ΔG for non-tritium containing hydrogen molecules can be obtained from *J. phys. chem Ref. Data*, Vol 14, suppl. 1, 1985 pg. 991,1211. For tritium containing molecules, the Gibb's free energy and equilibrium constants must be determined from the partition function. Due to the radioactivity of tritium, the standard form of the partition can not be used. Corrections need to be made.[4]

In order to expand known values to all possible temperatures, it is necessary to determine an equation that fits the data or to perform interpolation and extrapolation. Iterative non-linear interpolation can give greater accuracy, however, it has the disadvantage of taking longer to calculate. The iterative technique which I have used is Nevil's non-linear interpolation method.[5]

IV. EQUILIBRIUM EQUATIONS

In order to determine the equilibrium concentration of hydrogen isotopes, it is necessary to consider the reactions:

$$HD \longrightarrow \frac{1}{2}H_2 + \frac{1}{2}D_2$$

$$HT \longrightarrow \frac{1}{2}H_2 + \frac{1}{2}T_2$$

$$DT \longrightarrow \frac{1}{2}D_2 + \frac{1}{2}T_2$$

$$\frac{1}{2}H_2 \longrightarrow H$$

$$\frac{1}{2}D_2 \longrightarrow D$$

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[3] Levine, **Physical Chemistry** P. 166.

[4] Souers,**Hydrogen Properties for Fusion Energy**, Pg 20-24,160,295

[5] Burden, **Numerical Analysis**, P. 97

$$\frac{1}{2}T_2 \longrightarrow T$$

Using the above reaction equations it is possible to derive the following equilibrium equations

$$K_{X,H} \equiv \frac{X_H}{\sqrt{X_{H_2}}} \qquad K_{X,HD} \equiv \frac{\sqrt{X_H X_D}}{X_{HD}}$$

$$K_{X,D} \equiv \frac{X_D}{\sqrt{X_{D_2}}} \qquad K_{X,HT} \equiv \frac{\sqrt{X_H X_T}}{X_{HT}}$$

$$K_{X,T} \equiv \frac{X_T}{\sqrt{X_{T_2}}} \qquad K_{X,DT} \equiv \frac{\sqrt{X_D X_T}}{X_{DT}}$$

These reaction diagrams and equations do not include all possible components, however, they do include all components which occur in quantities which can effect normal muo-fusion reaction conditions.[6]

It is necessary to evaluate the initial concentrations of the isotopes.

$$X_{H_2} = X_{i,H} - \frac{1}{2}X_H - \frac{1}{2}X_{HD} - \frac{1}{2}X_{HT}$$

$$X_{D_2} = X_{i,D} - \frac{1}{2}X_D - \frac{1}{2}X_{HD} - \frac{1}{2}X_{DT}$$

$$X_{T_2} = X_{i,T} - \frac{1}{2}X_T - \frac{1}{2}X_{HT} - \frac{1}{2}X_{DT}$$

where $X_H, X_D, X_T, X_H, X_D, X_T, X_{HT}, X_{DT}$ and X_{HD} are the equilibrium concentrations, and $X_{i,H}, X_{i,D}$ and $X_{i,T}$ are the initial molecular concentrations of H_2, D_2 and T_2 respectively.

K_x is the molar equilibrium constant and can be calculated from the equilibrium pressure constant K_p.[7] Assuming Ideal gas behavior $K_p = K_{eq}$.

$$K_x = P^{-\Delta n} K_{eq}$$

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[6] Gill, **Tritium Handling in Vacuum Systems,** Los Alamos National Lab (1983), P. 20.

[7] Lewis, **Thermodynamics**, pp. 169–175.

At temperatures less than 2000 K, when only D_2,DT and T_2 are present many of the terms in the above equations approach zero. It is then possible to obtain a quadratic equation which can be used to solve the above equilibrium equations. **Care must be taken,** however, since when K_x becomes large, loss of significant figures due to rounding error makes it impossible to get accurate results using the normal form of the quadratic formula. Accurate approximations can be obtained using numerical methods of solution.

When protium, deuterium and tritium are present, the solution of the equilibrium equations becomes more complicated, especially at high temperatures. In order to analyze the full effects of manipulating reaction conditions, it is necessary to have a method of solution which will work when all reaction components are present. Newton's method[8] of solving systems of non-linear equations is a quadratically converging iterative technique which works well with these equations. Convergence can be speeded by decreasing the number of equations and unknowns. This can be done by combining the above equilibrium equations to form the following three equations:

$$X_{H_2} = X_{i,H} + \frac{K_H\sqrt{X_{H_2}}}{2} + \frac{K_{HD}\sqrt{X_{H_2}X_{D_2}}}{2} + \frac{K_{HT}\sqrt{X_{H_2}X_{T_2}}}{2}$$

$$X_{D_2} = X_{i,D} + \frac{K_D\sqrt{X_{D_2}}}{2} + \frac{K_{HD}\sqrt{X_{H_2}X_{D_2}}}{2} + \frac{K_{DT}\sqrt{X_{D_2}X_{T_2}}}{2}$$

$$X_{T_2} = X_{i,T} + \frac{K_T\sqrt{X_{T_2}}}{2} + \frac{K_{HT}\sqrt{X_{H_2}X_{T_2}}}{2} + \frac{K_{HT}\sqrt{X_{D_2}X_{T_2}}}{2}$$

When using Newton's method to solve the equilibrium equations some problems could result if special care is not taken. The equations should be solved in terms of X_{H_2}, X_{D_2} and X_{T_2} or in terms of X_{HD}, X_{HT} and X_{DT}, not in terms of X_H, X_D and X_T. When solved in terms of free H, D and T atoms, convergence is slow, and in some cases does not occur.

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[8] Burden, pp. 498–499.

V. SOLUTION OF DIFFERENTIAL KINETIC EQUATIONS

The differential kinetic equations presented in this paper are all linear and can therefore be solved using eigenvectors. The exact solution is, however, difficult to obtain, and is difficult to alter as new, more accurate factors are determined. It is therefore desirable to have a numerical method of solution which can be altered easily. The method I have used is the forth order Runge-Kuta method for systems of equations. [9]

The results obtained are equivalent to those published earlier with one marked exception. The reaction rate of muon catalyzed fusion can be expected to make an increase near 1500 K due to the presence of the free T and D radicals. The reactions:

$$1)\quad D + \mu \longrightarrow d\mu + e^-$$

$$2)\quad T + \mu \longrightarrow t\mu + e^-$$

$$3)\quad d\mu + T \longrightarrow t\mu + D$$

are expected to proceed much more rapidly than do the competing reactions:

$$D_2 + \mu \longrightarrow d\mu + D + e^-$$

$$T_2 + \mu \longrightarrow t\mu + T + e^-$$

$$DT + \mu \longrightarrow d\mu + T + e^-$$

$$DT + \mu \longrightarrow t\mu + D + e^-$$

$$d\mu + T_2 \longrightarrow t\mu + D + T$$

$$d\mu + DT \longrightarrow t\mu + 2D$$

These predictions are made acording to electron shell stability and calculations preformed by Johann Rafelski.[10] At low temperatures the slowest initial reactions which normally occur are those which contain DT. DT reacts more slowly than D_2 and T_2 in rate determining steps.[11] Recent predictions of Mel Leon and data analyses performed by Al Anderson indicate that at high temperatures (above ≤ 500 K) DT reacts faster than D_2 or T_2. In order to optimize reaction conditions it is necessary to vary DT concentration and to have free D and T atoms present in the reaction chamber.

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[9] Burden, pp. 225, 264.

[10] Rafelski, personal conversations

[11] Jones, pp. 127–133.

In most muon–catalyzed fusion cycles the transfer rate of $d\mu$ to $t\mu$ is a rate determining step (one of the slowest steps in the reaction chain), and is therefore important to the overall fusion rate.

Rate limiting reactions:

$$d\mu + D_2 \longrightarrow dd\mu d$$

$$d\mu + DT \longrightarrow dd\mu t$$

$$d\mu + DT \longrightarrow t\mu + 2D$$

$$d\mu + T_2 \longrightarrow t\mu + T + D$$

$$t\mu + D_2 \longrightarrow dt\mu d$$

$$t\mu + T_2 \longrightarrow tt\mu t$$

$$t\mu + DT \longrightarrow tt\mu d$$

$$t\mu + DT \longrightarrow dt\mu t$$

$$d\mu + T \longrightarrow t\mu + D$$

As can be seen from the above equations, most of the rate limiting steps are independent of the concentration of T. As the concentration of D and T increases, the concentration of the reactants of many of the rate limiting step decrease. Many of the rate determining steps will therefore be hindered by a large excess of free D and T atoms. In order to determine the exact concentrations necessary to optimize reaction conditions it will be necessary to have more accurate determinations of rate constants than now exist*.

VI. METHODS OF ALTERING KINETICS

In order to increase the reaction rate, it is necessary to alter the concentration of reaction components. This can be done in several ways with varying degrees of efficiency. Through the use of electromagnetic radiation, it may be possible to destroy undesirable molecules, thus freeing muons and reaction components to react in desired manners. It may also be possible to speed reaction rates through the use of radiation. A thorough investigation of the use of radiation in the above–mentioned manner has not yet been performed.

The most straightforward and perhaps optimual method of causing reactions to go in desired manners is to control the concentration of the components in a reaction chamber. In order to optimize reaction conditions, it is necessary to control the concentration of DT in reaction chambers. This can be done in several ways.

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* These rate constants are constant with respect to concentration. They are not constant with respect to temperature or pressure.

At low temperatures it is possible to run muon–catalyzed fusion reactions with non-equilibrated mixtures of D_2 and T_2 there–by retarding the interference due to DT molecules. As the temperature is raised, however, equilibrium is quickly reached. The equilibrium concentration of DT is temperature dependant and reaches a maximum ~ 50% at temperatures ~ 1500 K (considering equal consentrations of deuterium and tritium). The concentration of DT remains near constant at ~ 50% between 1500 K and 3000 K, then the concentration drops. This drop in DT concentration is due to the competing reactions:

$$D_2 \longrightarrow 2D$$

$$T_2 \longrightarrow 2T$$

$$DT \longrightarrow D + T$$

Another method of controlling DT within a reaction chamber involves selective laser-induced breakdown.[12] Lasers tuned to the proper vibrational frequency can selectively dissociate molecules while leaving other molecules unaffected. The principle disadvantage to eliminating DT in this manner appears to be the need of having an optical window in the reaction chamber. Although a need for an optical window is a disadvantage, it will not prevent this method from being used effectively. Further research needs to be performed in order to explore all the possibilities of this process.

A method of separating isotopes within a reaction chamber which could be used is absorption of gases on synthetic zeolites.[13] The hydrogen isotopes are absorbed by the zeolite, which is then heated slowly. The various molecular species come off at different temperatures, thus allowing the gases to be separated. This process has three main advantages over most other methods which could be used to separate gases within a reaction chamber. One advantage is that it can be used to remove helium from the chamber. This will be necessary when using reactors for long periods of time. Another advantage is that the method can be designed to operate without the use of a flow system. The use of flow systems increases the possibility of gas leakage. A third advantage of using zeolites to separate gases in a chamber is that it is relatively inexpensive to operate and maintain. The principle disadvantage of using zeolite absorption to seperate gases is that the process cannot be performed while reactions are taking place.

Two methods of isotope separation which are often coupled together are thermal diffusion and gas chromatography. [14] The coupling of these processes have the disadvantage that they require a flow system. These methods have many advantages, however, which far outweigh this one disadvantage. One advantage is

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[12] Blazejowski, **Applied Physics B.** 41, pp. 109–117.

[13] Aledseev, **Atomnaia Energia** vol. 54, No. 6, pp. 409–411.

[14] Takayasu, **Kenkyu Hokoku — Toyama Daigaku Torichumu Kagaku Senta**, vol. 2, pp. 45-52.

that separation can be obtained in a relatively short period of time. Gas chromatographs have been designed which can separate large quantities of hydrogen isotopes in as little as one minute. By coupling a thermal diffusion column to the gas chromatograph a yield of near 100% separation of the desired isotopes can be obtained. Another advantage of this method is that ortho and para isotopes can be separated. Ortho and para isotopes have been postulated to have different fusing rates. If this proves to be true, they will need to be separated in-order to optimize reaction conditions. A third advantage of this process is that it can be used to eliminate helium from a reaction chamber as can the method of absorption on synthetic zeolites.

Another process which can be successfully coupled with a gas chromatograph is isotopic thermal decomposition.[15] This process occurs when gases are run over hot metal at temperatures near 1,000 K. When DT, which can be separated using a gas chromatograph, is run through a column containing hot metals it decomposes into D and T atoms, then recombines in an equilibrated mixture of DT, D_2 and T_2. This mixture can be run through the gas chromatograph and the desired components removed. The metals which appear to work best for this process are uranium, thallium and palladium.

Other methods of isotope separation which could be applied to systems of nuclear fusion are pulse-transient gas diffusion, D.C. gas discharge, and low temperature distillation. None of these processes offer advantages over those which have been discussed above.

VII. CONCLUSIONS

In order to accurately determine the optimum reaction conditions for muon catalyzed fusion it is necessary to consider the concentration and the reaction rates of D, T, D_2, T_2 and DT as well as the concentration of any impurities in the reaction chamber.

The use of numerical methods to solve equilibrium and kinetic equations predicted to occur during muon catalyzed fusion makes it possible to easily test the effects of altering reaction conditions and to alter reaction equations as more accurate data is determined. Newton's method of solving non-linear systems of equations is a quadratically converging method of solution which works well for solving equilibrium equations encountered while working with muo-fusion. The Runge-Kuta method of solving systems of first order differential equations is an easily modifiable method of solution which can be applied to muo-fusion rate equations.

Solution of muon catalyzed fusion rate equations indicates that an increase in the fusing rate should occur above 1500 K due to the presence of free T atoms in the reaction chamber.

In order to optimize reaction conditions it is necessary to control the concentration of DT in the reaction chamber. The most promising methods of controlling DT

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[15] Masakazu, **J. Appl. Radiat. Isot.** vol. 34, No. 4, pp. 687–691.

concentration appear to be laser-induced breakdown of the DT molecule, absorption and removal using synthetic zeolites, or gas chromatographic separation coupled with a thermal diffusion column or an isotopic thermal decomposition chamber.