PROCEEDINGS OF SCIENCE

GEANT4 Simulation Package for Interactions Related to Muonic Atoms and Muon-Catalyzed Fusion (μCF)

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The muon-catalyzed fusion (μCF) is an established method in which D-T reactions occur at low temperatures (at or below room) and pressure. The reduced size of diatomic muonic molecules (say ddμ or dtμ) allows fusion to occur due to the greatly enhanced wave-function overlap. Under the current dMu/DT collaboration, an attempt is being made to study the μCF rate and sticking fraction at a relatively higher temperature (but $< 3 \times 10^3$ K) and pressure (but $< 10^5$ bar), using a diamond anvil cell with D-T mixture. In parallel, physics processes related to formation, transport, isotopic transfer, and other de-excitation processes of muonic atoms as well as μCF and reactivation of muons to the fusion cycles are being modeled in GEANT4. This article describes the current status of physics process modeling of μCF in GEANT4.

41st International Conference on High Energy physics - ICHEP2022,
6-13 July 2022
Bologna, Italy

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PoS(ICHEP2022)1232

1. Introduction

Muons, after stopping in D-T mixtures, form muonic atoms (dμ, tμ), which further produce diatomic muonic molecules (ddμ, dtμ, ttμ). The larger mass of the muon in comparison to the electron (207 times) reduces the molecular size, increasing the Coulomb screening between the nuclei and hence enhancing the nuclear wave function overlap and induces a fusion event. Several fusion reactions and their products have been shown in equations 1-3.

$$dt\mu- > \alpha\mu + n \text{ (sticking) or } dt\mu- > \alpha + \mu + n \text{ (no sticking), yield : 14.1MeV} \quad (1)$$

$$dd\mu- >^3 \text{He}\mu + n \text{ (sticking) or } dd\mu- >^3 \text{He} + \mu + n\text{(no sticking), yield : 3.3MeV} \quad (2)$$

$$tt\mu- > n + n + \alpha\mu \text{ (sticking) or } tt\mu- > n + n + \alpha + \mu\text{(no sticking), yield : 11.3MeV} \quad (3)$$

The probability of occurrence and rate of fusion reaction varies with the muonic molecules concerned; for instance, dtμ fusion rates ($1.3\times10^{12}\,\text{s}^{-1}$) are faster than dd$\mu$ ($4\times10^{8}\,\text{s}^{-1}$). Nevertheless, these are much faster than the molecule formation rates ($\sim 10^2 - 10^4$ times) in all cases [1]. Hence, theoretically, the μCF cycles would continue until the μ^- decays (muon lifetime: 2.2 μs). However, with a probability of initial sticking fraction (ω_s^0< 1%), μ^- sticks to one of the byproducts of fusion, like α or ^{3}He. It has also been observed that with a probability 'R', it is reactivated from this undesirable bonding by the scattering of muonic alpha with other atoms/nuclei in the D/T mixture, and this process is called stripping. In this process, the net loss fraction due to sticking can be expressed as ω_s^{eff} as shown in equation 4. The total fusion yield (Y_f) is estimated by equation 5. Here, $\lambda_0 = 1/(\mu^-$ lifetime) $= 0.455\times10^6\ \text{s}^{-1}$, λ_c is the average time between fusions, also called the muon cycling rate, and φ is the fuel density relative to liquid hydrogen density, LHD (4.25×10^{22} atoms cm^{-3}).

$$\omega_s^{eff} = \omega_s^0(1 - R) \quad (4)$$

$$Y_f \simeq (\omega_s^{eff} + \frac{\lambda_0}{\lambda_c\varphi})^{-1} \quad (5)$$

The fusion yield and cycling rate have been estimated theoretically as well as experimentally by several groups and the common goal is to achieve break-even by increasing Y_f and reducing ω_s^{eff} [2, 3]. In this article, we report an ongoing effort to model the involved physics processes in GEANT4 [4] and compare measured sticking fractions with established values in various conditions of temperatures, and fuel density. The simulation framework uses some pre-existing physics processes in GEANT4 along with new classes to simulate Muon stopping -> Muonic atom formation -> Muonic atom transfer -> Diatomic muonic molecule formation -> Muon catalyzed fusion -> stripping & Reactivation. The simulation is being carried out to support the experimental design of the diamond anvil cell μCF chamber [5], and consider D:T= 50:50 as fuel target.

2. Physics Process Models for Muonic Atom & μCF designed in GEANT4

The stopping of muon and atomic capture is handled by `G4MuonMinusAtomicCapture`. Following the capture process, μ^- cascades down to lower atomic levels via several de-excitation mechanisms, such as inelastic scattering, Auger, radiative transitions, isotopic transfer, and muonic

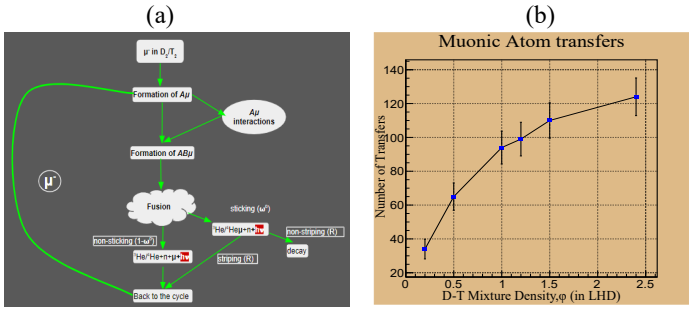

Figure 1: (a) Schematic drawing of Muon Catalyzed Fusion cycle. (b) Isotopic transfers ($d\mu \rightarrow t\mu$) with increase in density.

molecule formation and fusion. In the muonic atom isotopic transfer process, μ^- moves from a lightly-bound atom (say dμ) to a tighter one (tμ) via collision. A new class, `MuonicAtomTransfer` has been constructed which decides between this transfer and the elastic collision without transfer as shown in equation 6. The transfer rates are strongly dependent on the density of the fuel and concentration of atoms [3]. This new process has been designed based on the observed/calculated cross-sections.

$$\begin{aligned} d\mu + t &\rightarrow d\mu + t \text{ (scattering } :\sigma_{dd} \sim 2\times10^{-20}\text{cm}^2) \\ d\mu + t &\rightarrow t\mu + d \text{ (isotopic transfer } :\sigma_{dt} \sim 16\times10^{-20}\text{cm}^2) \end{aligned} \tag{6}$$

Afterward, in `MuonCatalyzedFusion` class, fusion processes have been implemented based on observed interaction rates and initial sticking probabilities data and their variations with D/T concentrations, fuel temperature and φ from [2, 3, 6]. In the case of sticking, $\alpha\mu$ and ^{3}Heμ have been emulated by ^{4}H derived using `G4IonTable` base class. This stand-in is a fair approximation given it has the same atomic mass and nuclear charge as muonic alpha. The reactivation of μ^- from $\alpha\mu$ and ^{3}Heμ, significantly increases the cycling rate and hence fusion yield. The cross-sections observed in [7] using ion-atom impact collisions, further scaled to proton numbers and electron number density have been used for stripping calculations. The muon stripping process can be understood from electron stripping of He+ and electron/muon mass ratio, which in turn translates to the ratio of radii of electronic-He and muonic-He. Finally, the muonic atoms left are decayed by `G4MuonicAtomDecay` process. This class considers both Decay In Orbit (DIO) and Nuclear Capture (NC) processes and calculates the decay interaction lengths in accordance with either process.

3. Simulation Results & Discussions

This article showcases results by varying parameters, such as temperature and density obtained from the monte-carlo simulations described above. The isotopic transfers depend on the ground-state population of muonic atoms [3], and therefore the collision energy (dμ, t) has a significant impact on isotopic transfers. This has been studied by varying density (φ) from 0.2-2.4 LHD. The number of transfers has been displayed in figure 1 (a). The stripping of μ^- is fundamentally dependent on the collision of muonic alpha with other atoms and molecules and hence ω_s^{eff} should reduce with φ. Densities, 0.1-2.4 LHD have been studied and compared to the results of [8]. Particularly, at

higher densities the trend fails to match; the result has been shown in figure 2 (a). Finally, the fusion yield for temperatures < 1500 K and φ: 0.2-1.4 LHD has been shown in figure 2 (b).

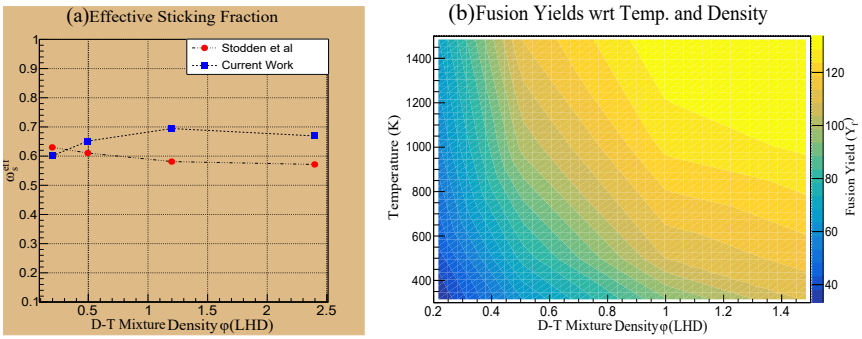

Figure 2: (a) Effective Sticking Fraction (ω_s^{eff}) with increase in density. (b) Simulation results for fusion yields (Y_f) for different temperatures and densities.

4. Summary

Different physics processes related to Muonic Atoms are being modeled in Geant4 based on the published interaction cross-section with fuel concentration, temperature and density effects. `MuonicAtomTransfer, MuonCatalyzedFusion,` and `MuonicAtomstripping` are some of the processes devised and integrated in the test code along with already existing muonic atom classes, like `G4MuonMinusAtomicCapture, G4MuonicAtomDecay`. Simulations are carried out for D:T = 50:50 mixture; rates for other concentrations of T are not implemented yet. The initial sticking fraction was considered to be 0.857 %. The results from this elementary simulation are promising and can be improved by implementing the cycling rates for tritium concentrations other than 50%. The lack of muonic atom interaction cross-sections creates difficulty in implementing alongstep/post-step reactions. These methods are essential for the implementation of a better model for energy loss and scattering of muonic atoms. This way, precise estimation of reactivation including stripping for excited state, simulation of hyperfine transitions of muonic atoms, etc can be added.

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