

NUMERICAL SIMULATION OF COMPOSITIONAL REDISTRIBUTION DRIVEN BY ISOTOPOLOGUE FRACTIONATION DURING SOLIDIFICATION OF D-T FUEL IN ICF TARGETS

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Cryogenic D-T fuel targets for inertial confinement fusion (ICF) are typically designed as spherical multilayered pellets. Structural defects in the solid D-T fuel layer can significantly degrade implosion efficiency [1]. However, isotopologue fractionation during solidification can introduce inhomogeneities in the solid D-T layer [2]. In this study, numerical simulations were performed to quantify the impact of isotopologue fractionation on the component distribution within the D-T target during solidification. The results indicate that fractionation gives rise to a radial gradient in isotope concentrations across the solid D-T layer, which in turn alters the equilibrium composition of the central D-T gas. The D-T ratio deviates from the optimal 50:50, reducing the theoretical upper limit of fusion reaction efficiency to as low as 64.2% at ignition. Insufficient isotope exchange further exacerbates this reduction in ignition performance.

A 3D model of a double-layered spherical D-T target was constructed. The target model consisted of an inner D-T gas core and outer liquid D-T layer, as shown in Figure 1. Tetrahedral elements were employed for the mesh, with enhanced refinement near critical boundaries to ensure numerical stability and accuracy. To simplify the mathematical model, the simulations assumed laminar, incompressible flow of the liquid D-T, and ignoring gravitational effects. The accumulation of kinetic fractionation during nonequilibrium solidification leads to macrosegregation. Therefore, a simulation framework was developed in ANSYS Fluent (ANSYS, Inc.), a widely used commercial computational fluid dynamics (CFD) software [3], that couples heat transfer, species transport, and solidification–melting physical model to investigate the compositional distribution of D-T mixtures during solidification induced by macrosegregation [4].

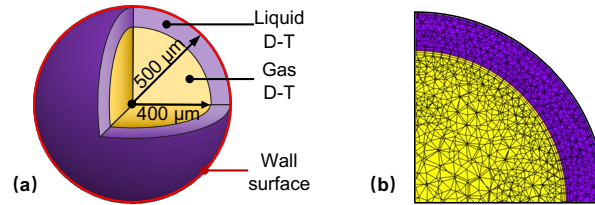


Figure 1. (a) Geometry of 3D spherical D-T target (b) Mesh of spherical D-T target.

At cryogenic temperatures, isotopic exchange reactions drive the mixture toward an equilibrium composition of approximately D_2 : DT : T_2 = 3:4:3 [5]. Solidification was initiated by gradually reducing the wall surface temperature from 19.7 K to 19 K, establishing a radial thermal gradient that promoted inward solidification. Simulation results revealed pronounced macrosegregation within the solid D-T layer, as shown in Figure 2. At the onset of solidification, T_2 was preferentially incorporated into the solid phase, whereas D_2 was progressively enriched in the remaining liquid. Consequently, a distinct radial gradient developed: the early solidified region near the outer wall exhibited the highest T_2 concentration, while the inner boundary region was enriched in D_2 . The mole fractions of molecules radially distributed inward from the outer surface of the solid D-T layer ranged from 0.293 to 0.397 for D_2 , 0.400 to 0.348 for DT , and 0.307 to 0.254 for T_2 , respectively.

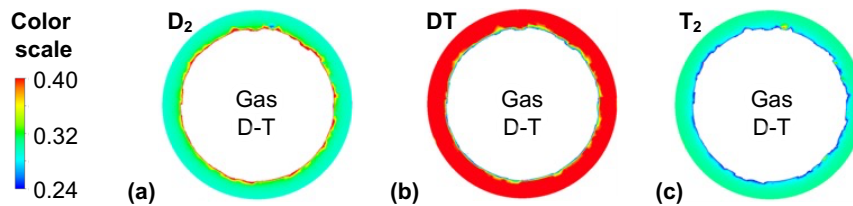


Figure 2. Compositional distribution in cross-section of D-T layer. (a) D_2 distribution, (b) DT distribution, (c) T_2 distribution.

Initially, the target pellet is filled with a 1:1 molar mixture of D_2 and T_2 gas. Owing to the relatively short timescale of the layering process, complete isotopic equilibrium cannot be achieved. Consequently, the actual D_2 : DT : T_2 composition in the D - T mixture varies between 5:0:5 (no exchange) to 3:4:3 (complete equilibrium). Simulations were performed for these two limiting cases: a D_2 - T_2 (1:1) mixture and a D_2 - DT - T_2 (3: 4: 3) mixture. For the solid layer formed by the D_2 - T_2 mixture, the mole fractions of D_2 (or D atom) across the solid layer, radially distributed inward from the outer surface, ranged from 0.480 to 0.600. In contrast, for the D_2 - DT - T_2 mixture, the corresponding mole fraction of D atom varied from 0.493 to 0.571. Figure 3 compares the radial distribution of D atoms in both cases. In practice, the actual distribution in the solid D - T layer is expected to fall between these two bounds. Since the reaction rate of D - D / T - T fusion is several orders of magnitude lower than that of D - T fusion, any deviation from the ideal fuel composition ratio can jeopardize the fusion performance.

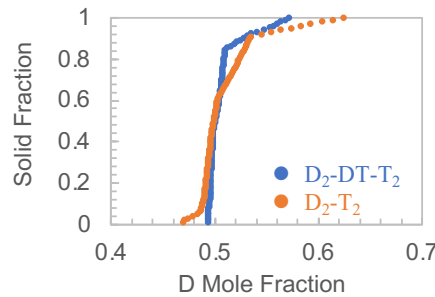


Figure 3. Radial profile of the D atom mole fraction from the outer surface of the solid D - T layer inward.

Furthermore, isotopologue fractionation induces a radial gradient in isotope concentrations within the solid D - T layer. These compositional variations in turn alter the equilibrium composition of the central D - T gas. To quantify this effect, the equilibrium mole fractions of gas components were evaluated applying Raoult's law and Dalton's law, based on the composition of the adjacent solid layer. The analysis revealed a shift in gas composition toward D_2 enrichment. Specifically, in the case of a solid D_2 - DT - T_2 layer, the gas-phase composition at the center was approximately 52.1% D_2 , 31.6% DT , and 16.3% T_2 , corresponding to a D atom fraction of 67.9%. For a solid D_2 - T_2 layer, the central gas-phase composition was approximately 75.6% D_2 and 24.4% T_2 . Overall, the molar fraction of D atoms in the D - T gas can vary from about 67.9% to 75.6%, which deviates significantly from the optimal 50:50 D - T ratio required to maximize fusion reactivity. Even at a D atom molar fraction of 67.9%, only 32.1% of D atoms can react with an equal fraction of T atoms to undergo D - T fusion reaction. The theoretical upper limit of fusion reaction efficiency is reduced to 64.2%. Moreover, the excess 34.8% of unreacted D atoms act as impurities, potentially hindering ignition and further decreasing overall reaction efficiency. Insufficient isotope exchange exacerbates this degradation in ignition performance.

In conclusion, this study presents a numerical investigation of isotopologue fractionation in D - T fuel during solidification within ICF target. The 3D simulations provide quantitative insights into how solidification affect species distribution, gas composition, and fusion performance. The results emphasize the critical importance of homogeneity for optimizing ignition and burn processes, and underscore the need for strategies to control or mitigate isotopologue fractionation during target fabrication. Decay heat introduces additional complexity to the phase-change process, which cannot be accurately captured by the current mathematical model, representing a limitation of this work. Overall, this work provides valuable insights for the improvement of D - T target preparation.

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